

TOUGH

Training Courses



Numerical Simulation of Nonisothermal Multiphase Flow Using TOUGH

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California, USA

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Subsurface models: then and now



- Result of abstraction
- Erroneous
- Occam's Razor:
*As complex as needed –
as simple as possible*

"A model of the Yanaizu-Nishiyama geothermal plant. Japan's 18 geothermal plants account for only 0.3 percent of its electricity production."

A. Pollack, Japan's Nuclear Future in the Balance, *New York Times*, May 9, 2011.

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A model is...

“... a *purposeful, simplified* representation of a real system”

“... a simple worldview with an attitude”

“*simple and with purpose*”:

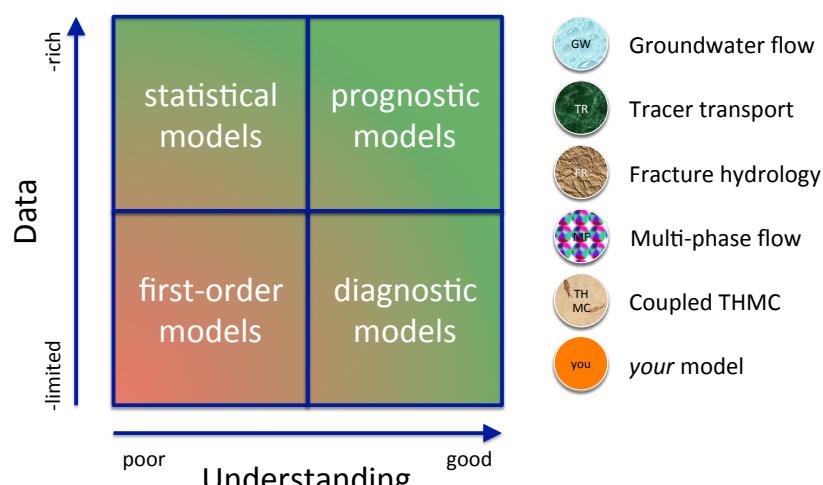
The model is *simple* in that it contains only features of *primary importance* for the *intended use* of the model

Occam's razor

“Non sunt multiplicanda entia praeter necessitatem”

Make it as complex as needed, ...
but *keep it as simple as possible!*

Models for the good and the bad, the **data** poor and the rich



after Holling (1978)

Role of Mathematical Modeling

TOUGH2
Improve process understanding
• Understand nonlinearities/coupled processes
• Evaluate non-observable quantities
• What-if scenarios (“virtual sandbox”)

iTOUGH2

Design experiments
• Identify experimental procedure yielding data that contain information about relevant properties

Analyze data
• Determine parameters from data
• Identify model structure

Decision support
• Risk assessment
• Sensitivity analysis

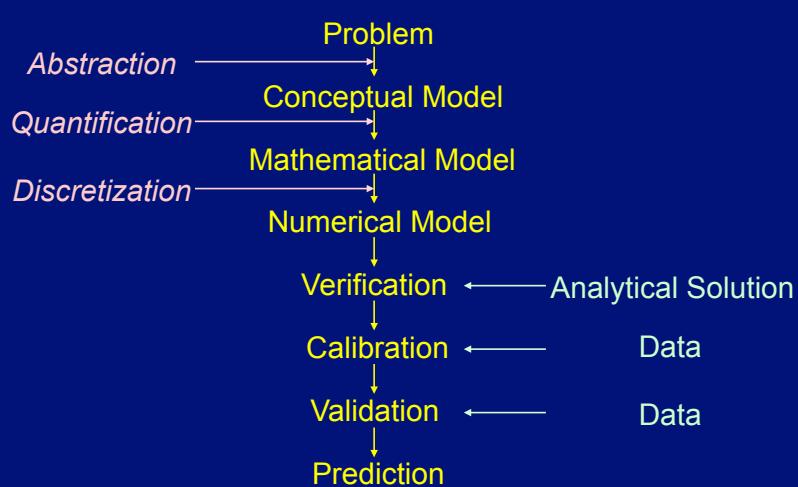
Make predictions
• Deterministic/probabilistic
• Sensitivity analysis

Uncertainty quantification

Optimization

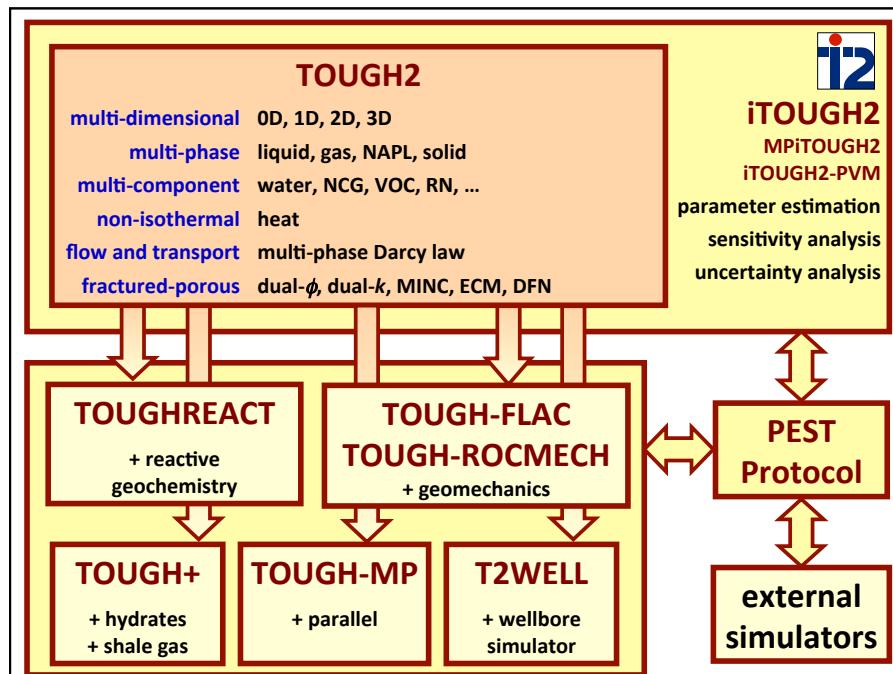
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Model Development



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Tools





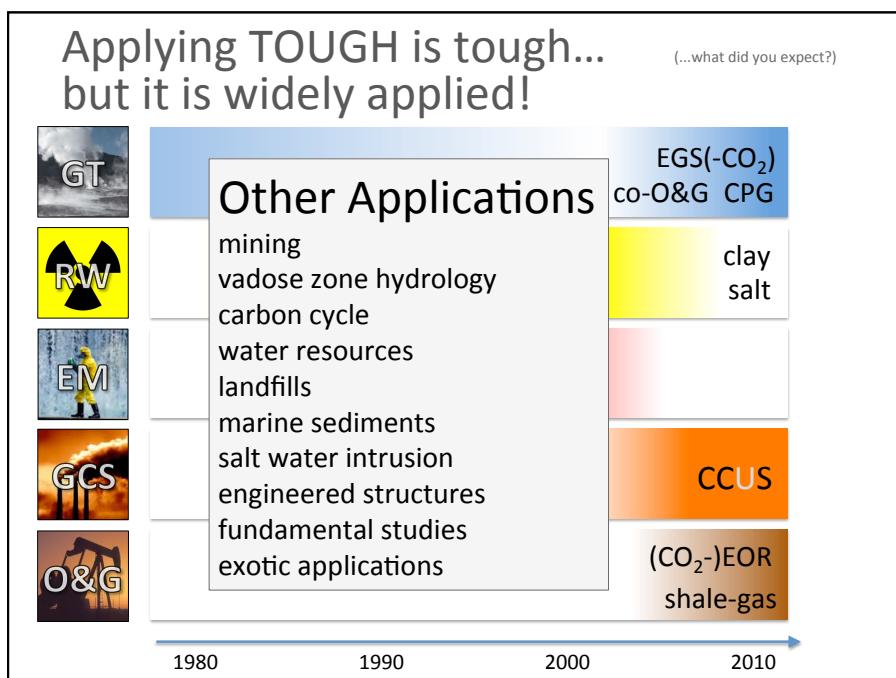
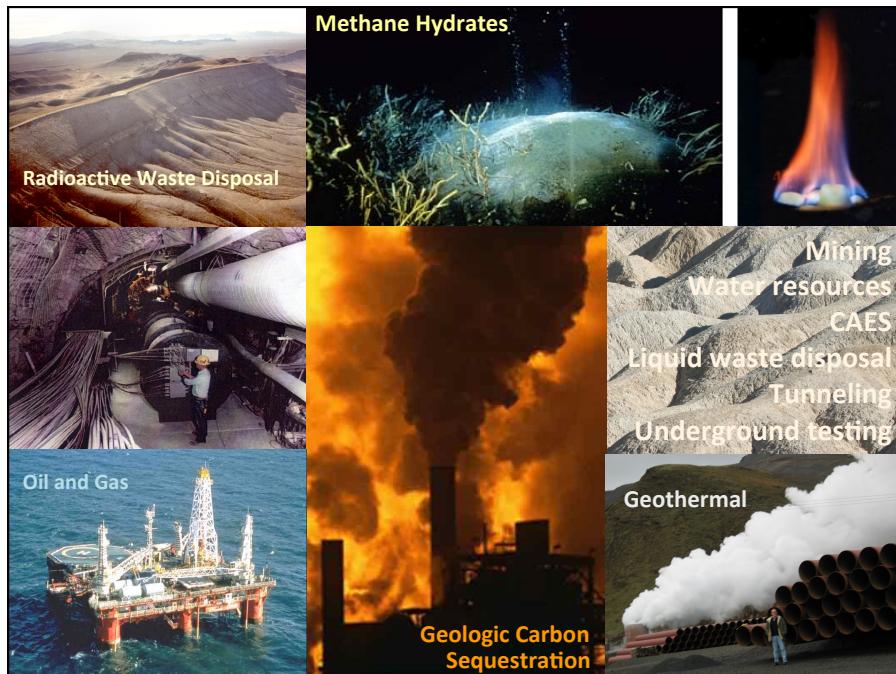
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Multiphase Flow Systems

Flow System	Phases	Components
groundwater aquifer	aqueous	water, solutes
vadose zone	aqueous gas NAPL	water, solutes air, vapor, CO ₂ , ... VOCs
geothermal reservoir	aqueous gas	water, solutes water vapor, NCGs
oil and gas reservoir	oil gas aqueous	alkanes, aromatics, solutes CH ₄ , NCGs, VOCs water, solutes

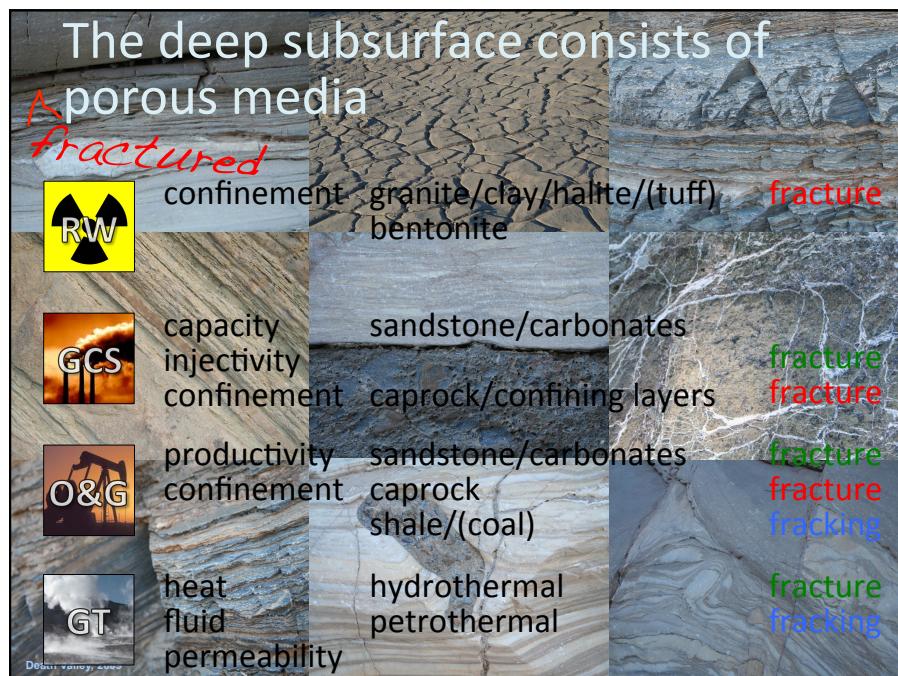
NAPL: non-aqueous phase liquids
VOC: volatile organic compound
NCG: non-condensable gas

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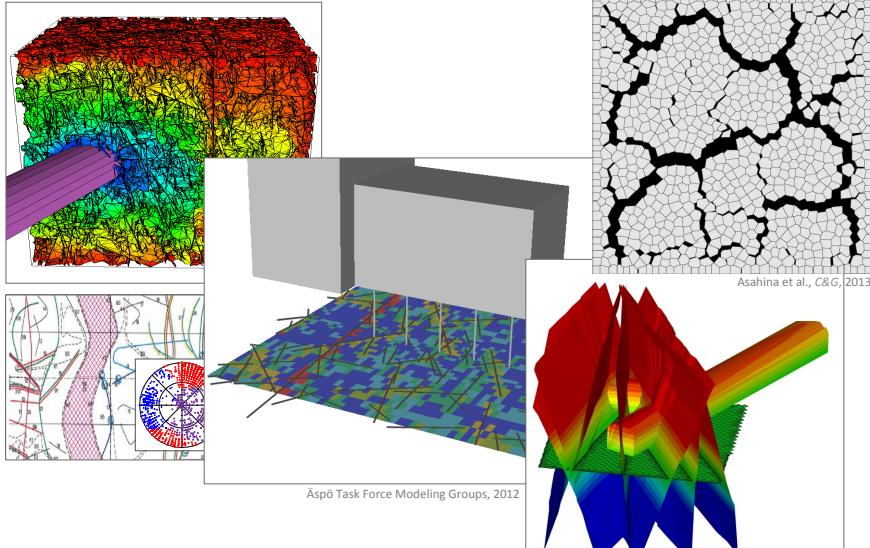


Different deep subsurface applications
are ~~different~~ *similar*

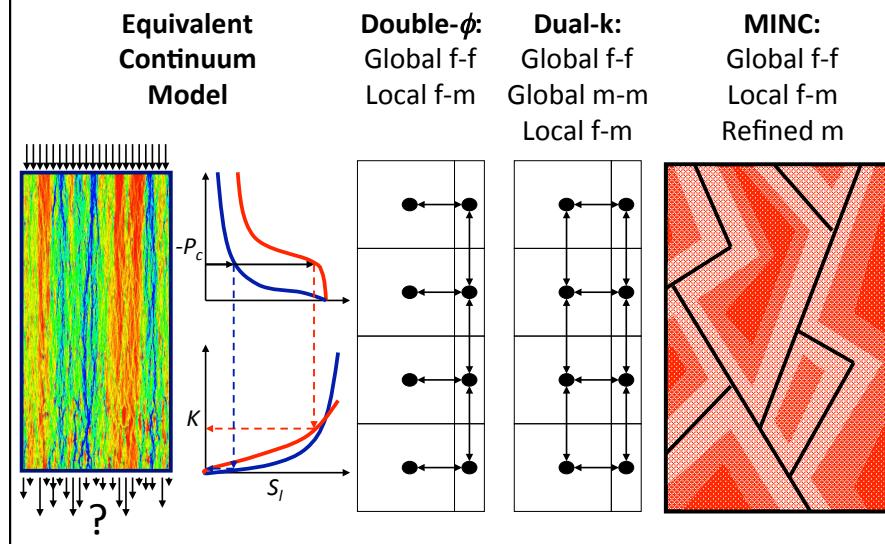
Activity	Driver	Mass	Time
 RW Retrievability	Env. & Safety Economics	10^4	10^6
 GCS Extraction	Env. & Safety Economics	10^{10}	10^3
 O&G Injection (EOR)	Economics Reservoir integrity	10^{10}	10^1
 GT Injection (EGS)	Economics Induced seismicity	10^{10}	10^1



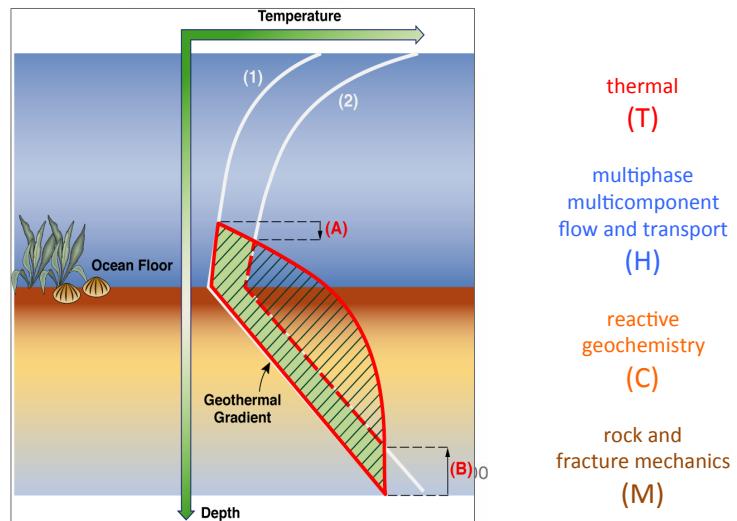
Discretely different fracture models ...



... or multiple-continua models



THCM coupled process modeling



Rock mechanics rocks the modeling world



Tectonic stability essential



Caprock integrity essential

Seismic events to be avoided



Seismic events induced by design

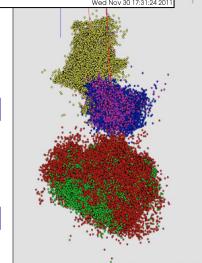
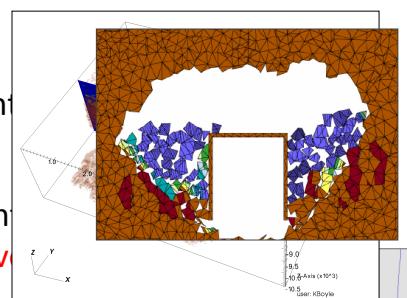
Fault reactivation to be avoided

Induced seismicity as monitoring tool

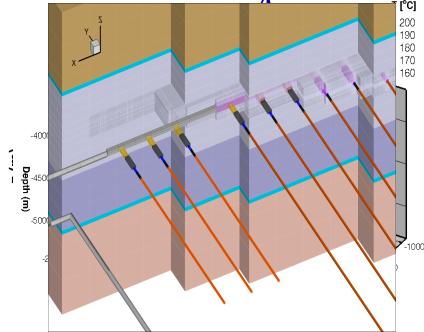
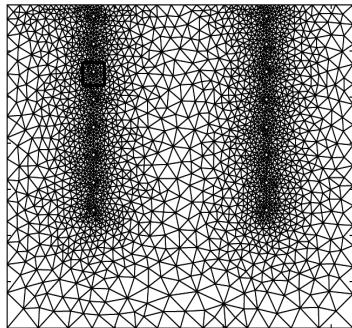


Seismic events induced by design

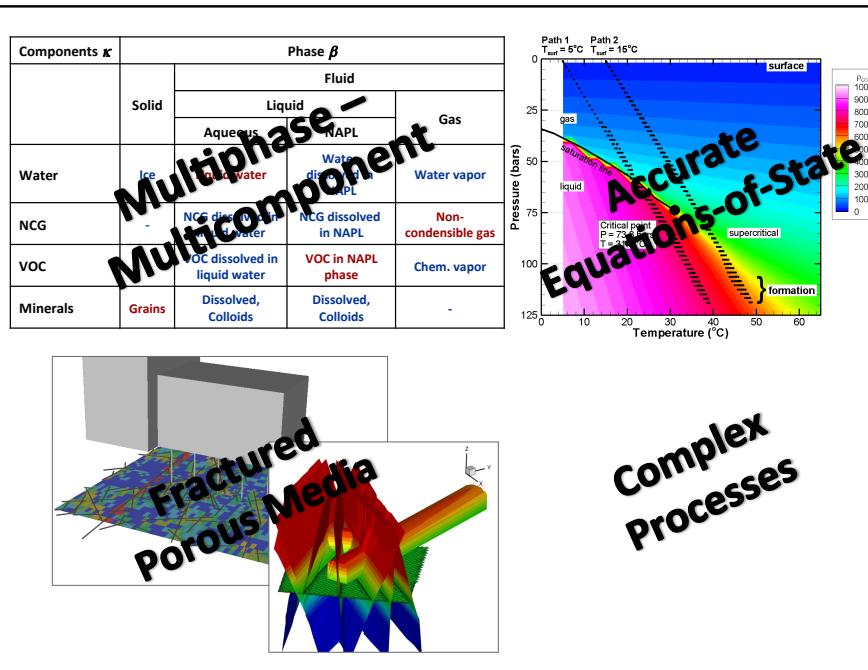
Induced seismicity as monitoring tool

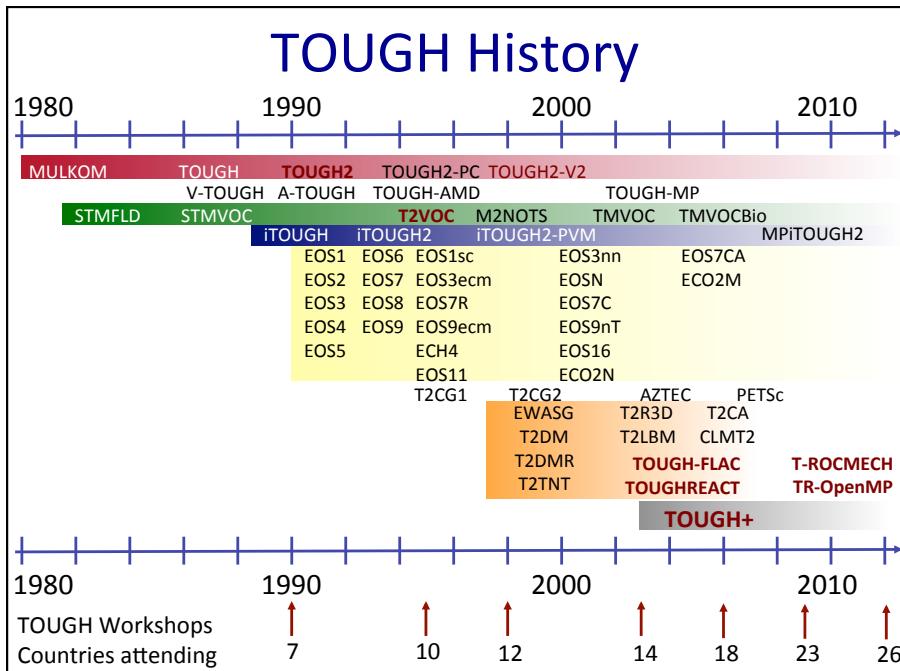


Natural or engineered system?



Engineered components affect natural system behavior
 Engineered components affect testing and monitoring data
 Engineered components may need to be explicitly modeled
 Engineered and natural systems may need to be fully coupled





Applications and Impact

- TOUGH family of codes installed in ~500 organizations in ~40 countries:
 - Academia
 - Government Organizations
 - Industry
- Applications in:
 - Geothermal
 - Nuclear Waste Isolation
 - Environmental
 - CO₂ Sequestration
 - Gas Hydrates
- Code development driven by research needs
- Strong support from active user community



Computers and Geosciences, 65(4), 2014
 Greenhouse Gases: Science and Technology, 3(6), 2013
 Transport in Porous Media, 90(1), 2011
 Computers and Geosciences, 37(6), 2011
 Vadose Zone Journal, 7(1), 2008
 Nuclear Technology, 164(2), 2008
 Energy Technology and Management, 28, 2007
 Geothermics, 33(4), 2004
 Vadose Zone Journal, 3(3), 2004

<http://esd.lbl.gov/TOUGH>

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TOUGH

$\frac{d}{dt} \int_{V_n} M^k dV_n = \int_{V_n} \mathbf{F}^k \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^k dV_n$

Software Documentation Licensing & Download Events User Support Search...

TOUGH Publications

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Publications per TOUGH Module:

Publications per Research Area:

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	Journal	Year	Citation	TOUGH Module	Research Area
1	Advances in Water Resources	2013	Castelletto, N., Testini, P., Gambolati, G., Bossie-Codreanu, D., Vincék, O., Daniel, J.M., Battistelli, A., Marcolini, M., Donda, F., and Volpi, V., (2013). Multiphysics modeling of CO ₂ sequestration in a faulted saline formation in Italy. <i>Advances in Water Resources</i> , doi: 10.1016/j.advwatres.2013.04.006.	TOUGH2	Carbon Storage
	International		Doeatash, J., Kowalsky, M.B., Doughty, C., Finsterle, S., Ajo-Franklin, J.B., Carrigan, C.R., Yang, X., Horváth,		

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TOUGH WIMP

The TOUGH Web Interface for Massive Parallelism—making parallel simulations easier than the command line since 2013.

Learn more Try it Now

CREATE EDIT MONITOR ORGANIZE

Organize

Job Name Status Time Queued Processors PBS Job ID Page: 1

Job Name	Status	Time Queued	Processors	PBS Job ID	Page: 1
Adv.dat	toberun	None	24		
inout	537 B	Jul 26, 2013, 04:09 PM	24		
INFILE	36.92 kB	Jul 26, 2013, 04:06 PM	24		
INFILE_ALLLOC	2.33 kB	Jul 26, 2013, 04:10 PM	24		
INFILE_LINQ	64.47 kB	Jul 26, 2013, 04:20 PM	24		
INFILE_PlotCore	0 B	Jul 26, 2013, 04:09 PM	24		
INFILE_PlotErr	10.67 MB	Jul 26, 2013, 04:21 PM	24		
INFILE_TS_HOME	11.82 kB	Jul 26, 2013, 04:20 PM	24		

Page: 2 Show All

Keep your simulation jobs organized with TOUGHWIMP's projects. Projects allow users to easily move between related groups of simulations without cluttering the screen with unnecessary buttons.

Download File ▾ Graph

Monitor your output directly in real time with TOUGHWIMP's web-based interface. With TOUGHWIMP's interface, users can easily keep track of their simulations and see the size and contents of their output files. With TOUGHWIMP's web-based tools, users can analyze the results of their simulation without the hassle of having to copy outputs to another program.

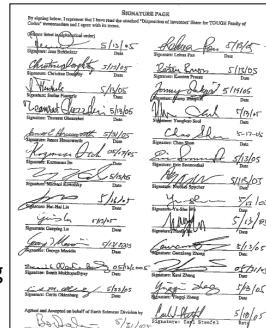
Tailing files

Live-Updating Graphs

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TOUGH Developers

Rick Ahlers	Karsten Pruess	Maryam Akhavan
Jens Birkholzer	Mathew Reagan	Alfredo Battistelli
Bo Bodvarsson	Jonny Rutqvist	Grimur Björnsson
Chris Doughty	Chao Shan	David Bullivant
Stefan Finsterle	Eric Sonnenthal	Ron Falta
Jeff Johnson	Nic Spycher	Yoojin Jung
Noel Keen	Haruko Wainwright	René Lefebvre
Mike Kowalsky	Yu-Shu Wu	Auli Niemi
George Moridis	Tianfu Xu	Mike O'Sullivan
Curt Oldenburg	Guoxiang Zhang	Torben Sonnenborg
Lehua Pan	Keni Zhang	Steve Webb
George Pau	Yingqi Zhang	Steve White
...



*Developer's share of licensing income donated
and reinvested into TOUGH developments*

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Course Objectives

- Understanding *concepts* and *physical processes* implemented in TOUGH
- Understanding *mathematical* and *numerical* methods implemented in TOUGH
- Understanding TOUGH *input and output*
- Understanding *model development* process
- Developing capability to solve scientific and engineering problems with TOUGH

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Course Outline

- Introduction
- Multiphase Flow Tutorial
- Governing Equations and Numerical Methods
- TOUGH Concepts
- TOUGH Input
- Computer Exercises:
 - Step-by-Step Model Development
 - Sample Problems
 - Problem Variations
- Discussions

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Multiphase Flow Tutorial

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

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Outline

- Notations and Definitions
 - Phase and Component
 - State Variables
- Governing Equations
 - Mass balance equations
 - Mass accumulation term
 - Flux term
- Equation-of-State
- Other Processes
 - Heat transfer
 - Radionuclide transport
 - Diffusion
 - Klinkenberg effect
 - Vapor pressure lowering

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Phases and Components

- Phase β

- Physical state (liquid/aqueous, gas, NAPL, solid)
- May consist of multiple components
- Separated by interface (immiscible → capillarity)
- Continuum with slowly varying thermophysical properties (density, viscosity, etc.)

- Component κ

- Chemical species (H_2O , “air”, CO_2 , $NaCl$, C_nH_{2n+2} , ...)
- Partitioned in multiple phases, determined by chemical potential and kinetics
- Conserved in closed system → mass balance equations

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Multiphase, Multicomponent

Components κ	Phase β			
	Solid (s)	Fluid		
		Liquid (l)	NAPL (o, n)	Gas (g)
Water	ice	Liquid water	Water dissolved in NAPL	Water vapor
Air	- (NCG)	Air dissolved in liquid water	Air dissolved in NAPL	Air as non-condensable gas
VOC	-	VOC dissolved in liquid water	VOC in NAPL phase	Chem. vapor
Minerals	Grains	Dissolved, Colloids	Dissolved, Colloids	Dust

- Gibbs' phase rule: $f = NK + 2 - NPH$, where f is number of degrees of freedom = number of intensive variables
- In a system with NPH phases, define $NPH-1$ phase saturations: $\sum_{\beta=1}^{NPH} S_{\beta} = 1$
- $f + NPH - 1 = (NK + 2 - NPH) + (NPH - 1) = NK + 1$
- Number of equations per grid block: $NK + 1$

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Phase Transition and Phase State

- **Phase transition:**

- Mass transfer of a *component* between *phases* (evaporation/condensation, dissolution/outgassing, freezing/thawing)
- Involves latent heat effects

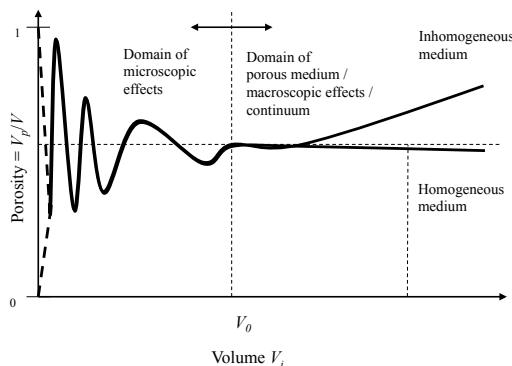
- **Phase state:**

- Single-phase (liquid/gas/NAPL); two-phase; three-phase
- In a closed system, the number, volume, and mass of a *phase* may change, but the mass of the *component* remains constant

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Key Assumptions

- *Continuum approach*
- *Local thermodynamic equilibrium*
- Representative elementary volume (*REV*)



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Notation and Definitions

Phase β	subscript β ($g = \text{gas}$; $l, a = \text{liquid, aqueous}$; $s = \text{solid}$; $sc = \text{supercritical}$; $n, o = \text{NAPL, oil}$; $w = \text{wetting}$; $nw = \text{non-wetting}$)
Component κ	superscript κ ($w = \text{water}$; $a = \text{air}$; $h = \text{heat}$; ...)
Porosity ϕ	$\phi = V_{\text{porespace}}/V_{\text{total}} = V_\phi/V$
Saturation S_β	$S_\beta = V_\beta/V_\phi = \theta_\beta/\phi$
Pressure P_β [Pa]	$P_\beta = P_{\text{ref}} + P_{c\beta}$ ($P_{\text{ref}} = P_g$; $P_c = P_l - P_g$)
Mass Fraction X_β^κ	$X_\beta^\kappa = m_\beta^\kappa/m_\beta = m_\beta^\kappa/(\sum_\kappa m_\beta^\kappa)$

Mass Conservation

$$\frac{\partial}{\partial t} \int_{V_n} M^\kappa dV_n = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^\kappa dV_n$$

M - "accumulation term" \mathbf{F} - "flow term" q - "sink/source term"

V_n : *volume* of arbitrary subdomain [m^3]

Γ_n : closed *surface* [m^2]

\mathbf{n} : normal vector on surface element $d\Gamma_n$, pointing inward into V_n .

M^κ : specific *mass* of component κ [kg m^{-3}]

\mathbf{F}^κ : specific *mass flux* of component κ [$\text{kg m}^{-2} \text{s}^{-1}$]

q^κ : specific mass *sink/source* [$\text{kg m}^{-3} \text{s}^{-1}$]

One equation for each component κ

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Mass Accumulation Term

- Mass balance equation [kg s⁻¹]

$$\frac{d}{dt} \int_{V_n} M^\kappa dV_n = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^\kappa dV_n$$

- Specific storage [kg m⁻³] Mass storage [kg]

$$M^\kappa \quad \int_{V_n} M^\kappa dV_n$$

- Mass accumulation term [kg s⁻¹]

$$\frac{d}{dt} \int_{V_n} M^\kappa dV_n$$

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Mass Storage

Specific pore volume:

$$\phi$$

Specific volume of phase β :

$$\phi S_\beta$$

Specific mass of phase β :

$$M_\beta = \phi S_\beta \rho_\beta$$

Specific mass of component κ in phase β :

$$M_\beta^\kappa = \phi S_\beta \rho_\beta X_\beta^\kappa$$

Total specific mass of component κ in all phases:

$$M^\kappa = \phi \sum_\beta S_\beta \rho_\beta X_\beta^\kappa$$

Total mass of component κ in volume V :

$$\int_V M^\kappa dV$$

Storage: The amount of mass present in a unit volume of the flow system

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Flow Term

- Mass balance equation [kg s⁻¹]

$$\frac{d}{dt} \int_{V_n} M^\kappa dV_n = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^\kappa dV_n$$

- Flux [kg s⁻¹ m⁻²] Flow rate Across interface [kg s⁻¹]

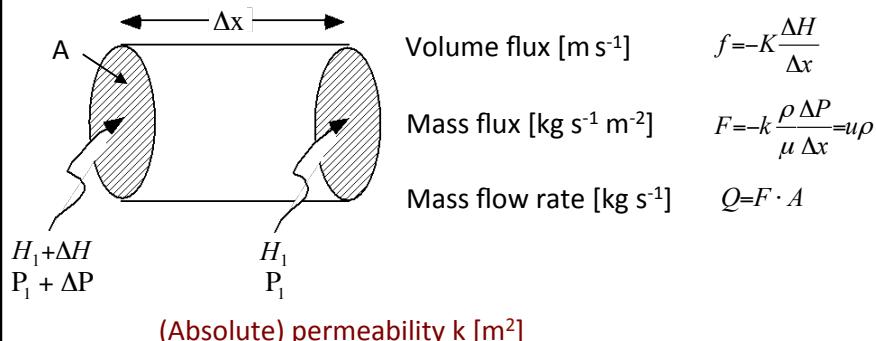
$$\mathbf{F}^\kappa \cdot \mathbf{n}$$

- Net mass flow into volume element [kg s⁻¹]

$$\int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma_n$$

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Darcy's Law (Henri Darcy, 1856)



$$Hydraulic conductivity [m/s]$$

$$K = k \frac{\rho g}{\mu}$$

$$Unsaturated hydraulic conductivity [m/s]$$

$$K_{rl} = k_{rl} \cdot K$$

$$1 \text{ darcy} \approx 10^{-12} \text{ m}^2 \approx 10^{-5} \text{ m/s}$$

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Multiphase Flow (phases: β = liquid, gas)

$$\mathbf{F}_\beta = -k \frac{k_{r\beta} \rho_\beta}{\mu_\beta} (\nabla P_\beta - \rho_\beta \mathbf{g})$$

- Fluid properties
 - Density ρ_β [kg m⁻³]
 - Dynamic viscosity μ_β [Pa s]
- Porous medium property
 - Absolute permeability k [m²]
- Interaction between fluids and porous medium
 - Relative permeability: $k_{r\beta}$ [-]
 - Phase pressure: $P_b = P_{ref} + P_c$; $P_{ref} = P_g$
 - Capillary pressure: $P_c = P_l - P_g = f(S_\beta)$

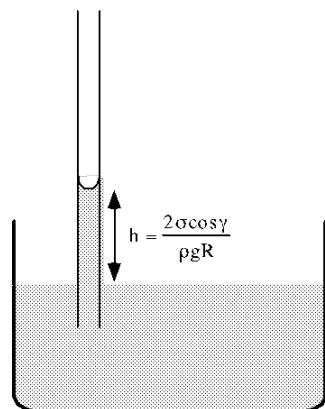
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Fluid and Porous-Medium Properties

- Fluid properties and laws
 - Density, viscosity, internal energy, surface tension
 - Function of pressure, temperature, (composition)
 - Ideal gas law, Henry's law, mixing laws
 - Provided internally → EOS modules
- Porous medium properties
 - Permeability, porosity, tortuosity, pore compressibility
 - Thermal conductivity, heat capacity, expansivity
 - Fracture spacing
- Interaction between fluids and porous medium
 - Relative permeability functions
 - Capillary pressure function

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Capillary Pressure



$$P_{cap} = \rho gh = \frac{2\sigma\cos\gamma}{R}$$

water

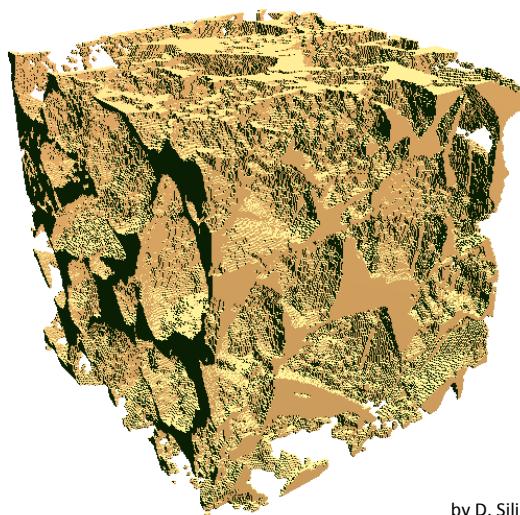
$\sigma(T = 20^\circ C) \approx 0.073 \text{ N/m}$; $\cos \gamma \approx 1$

for $R = 1 \mu\text{m} = 10^{-6} \text{ m}$ have
 $P_{cap} \approx 1.46 \times 10^5 \text{ Pa} = 1.46 \text{ bar}$

$\sigma(T = 250^\circ C) \approx 0.026 \text{ N/m}$

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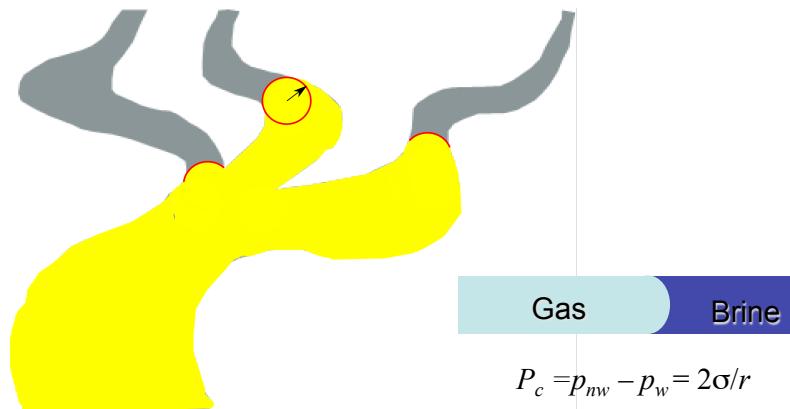
From Micro-CT to capillary pressure



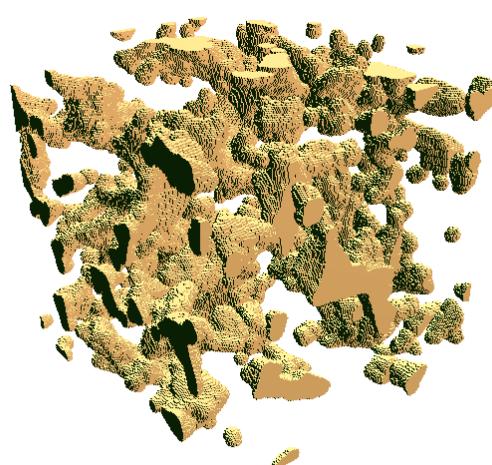
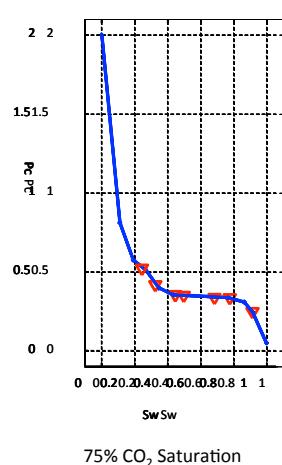
by D. Silin and T. Kneafsey 16

Maximum Inscribed Spheres

- Assumptions
 - Capillary equilibrium
 - Disperse saturation is negligible

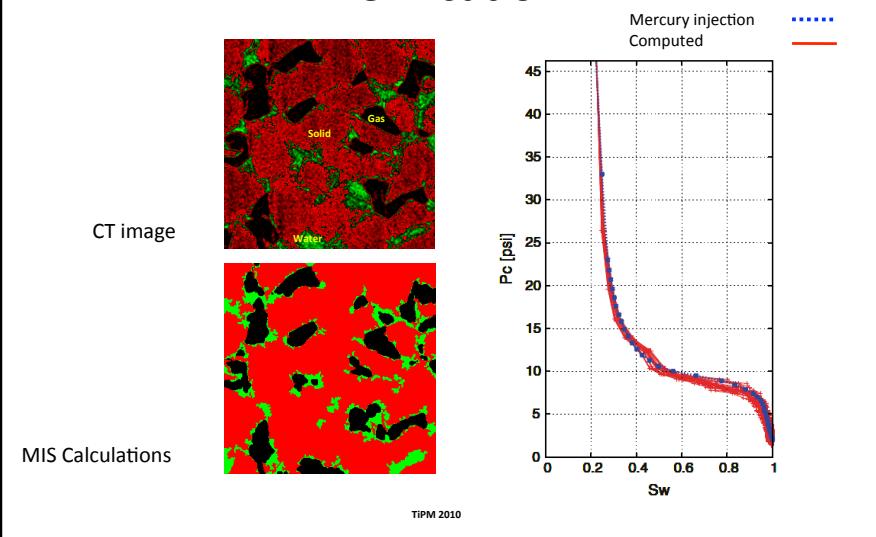


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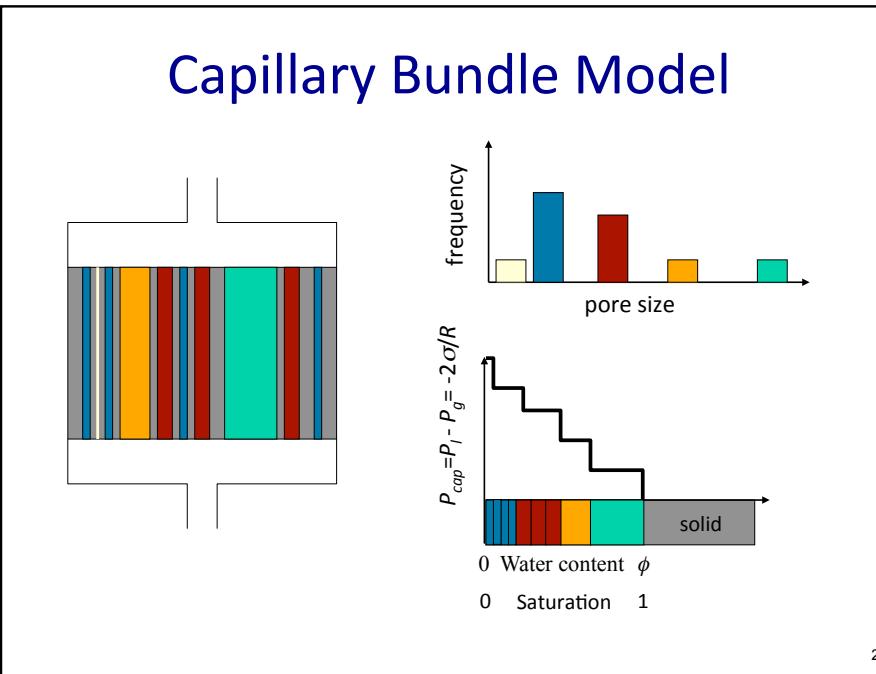


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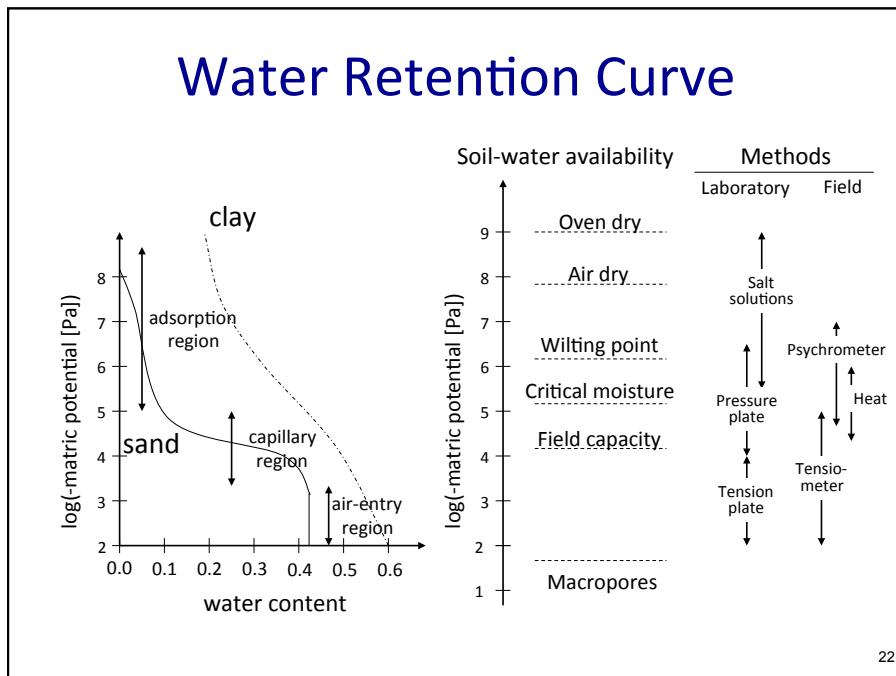
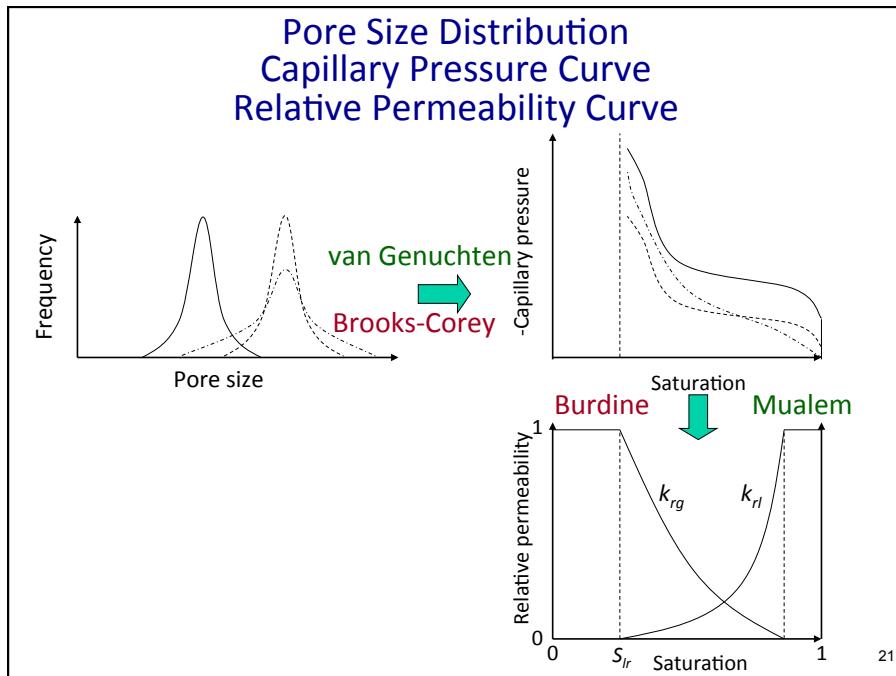
Maximal inscribed spheres: verification



Capillary Bundle Model



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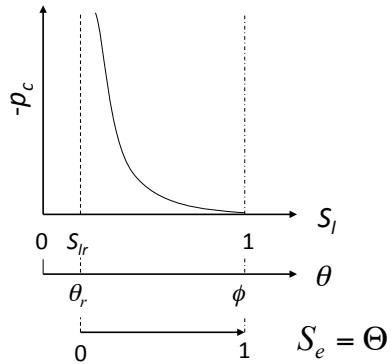
Effective Saturation, Water Content

Effective saturation

$$S_e = \frac{S_l - S_{lr}}{1 - S_{lr}}$$

Effective water content

$$S_e = \Theta \quad \Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{\theta - \theta_r}{\phi - \theta_r}$$



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Brooks-Corey (BC) Burdine

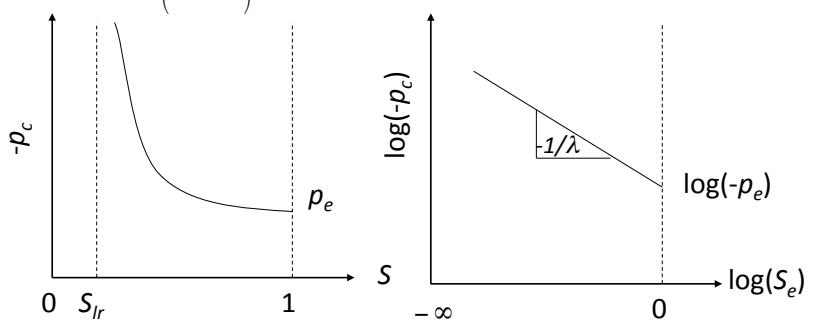
$$S_e = \left(\frac{p_e}{p_c} \right)^\lambda \rightarrow p_c = p_e \cdot S_e^{-1/\lambda}$$

$$k_{rl} = S_e^{\frac{2+3\lambda}{\lambda}}$$

$$k_{rg} = (1 - S_e)^2 \left(1 - S_e^{\frac{2+\lambda}{\lambda}} \right)$$

$\lambda > 0$ = pore-size distribution index

p_e = air-entry pressure



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van Genuchten (VG) Mualem

$$p_c = -\frac{1}{\alpha} \left[S_e^{-1/m} - 1 \right]^{1/n}$$

$n > 1$ (approx. $\lambda + 1$)

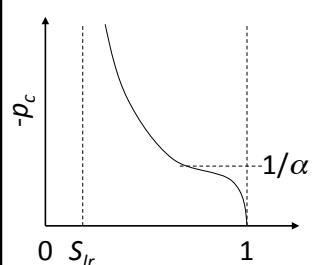
$$k_{rl} = S_e^\varepsilon \left[1 - \left(1 - S_e^{1/m} \right)^m \right]^2$$

$0 < m < 1; m = 1 - 1/n$

$$k_{rg} = (1 - S_e)^\gamma \left[1 - S_e^{1/m} \right]^{2m}$$

α^1 = inflection point (approx. p_e)

Pore connectivity: $\varepsilon = 1/2; \gamma = 1/3$



well-sorted soil →

small $\sigma \rightarrow$

large $n \rightarrow$

large $m \rightarrow$

flat curve

poorly sorted soil →

large $\sigma \rightarrow$

small $n \rightarrow$

small $m \rightarrow$

smooth, steep curve

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Relative Permeability

➤ Relative permeability: dimensionless number between zero and one

➤ Phase interference:

- for $S_\beta < 1$, not all pores are conducting phase $\beta \rightarrow$ conductivity depends on cross-section available for flow, i.e., saturation

- Large pores drain first → large reduction (Poiseuilles Law)

- Tortuosity increases → stronger reduction

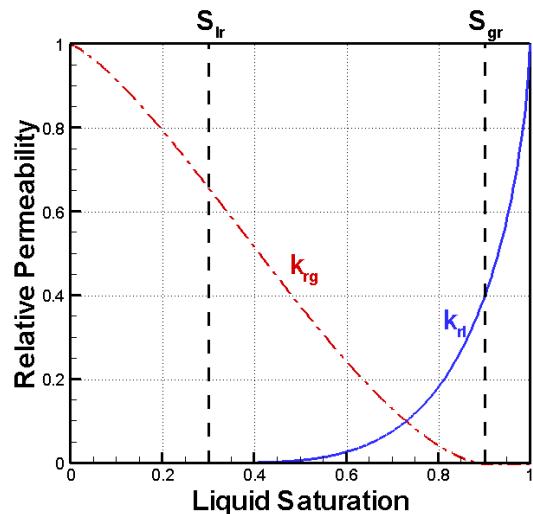
- At high suction, viscosity increases

- Film flow

$$0 \leq \sum_{\beta=l,g,o} k_{r\beta} \leq 1$$

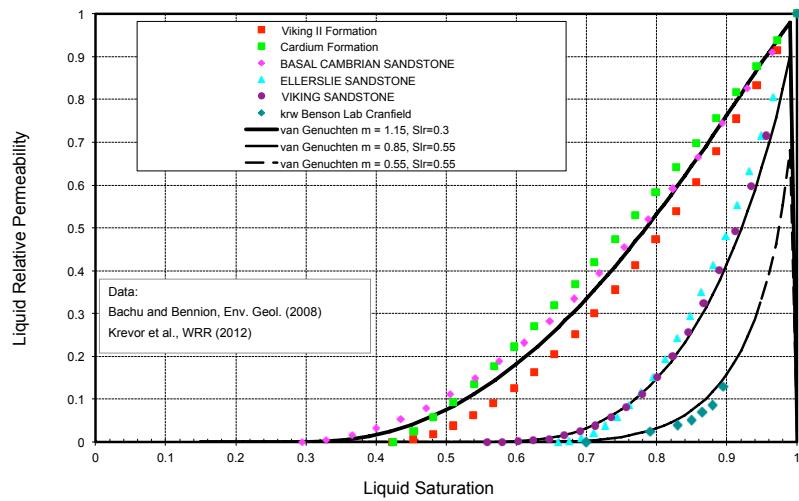
26

Relative Permeability

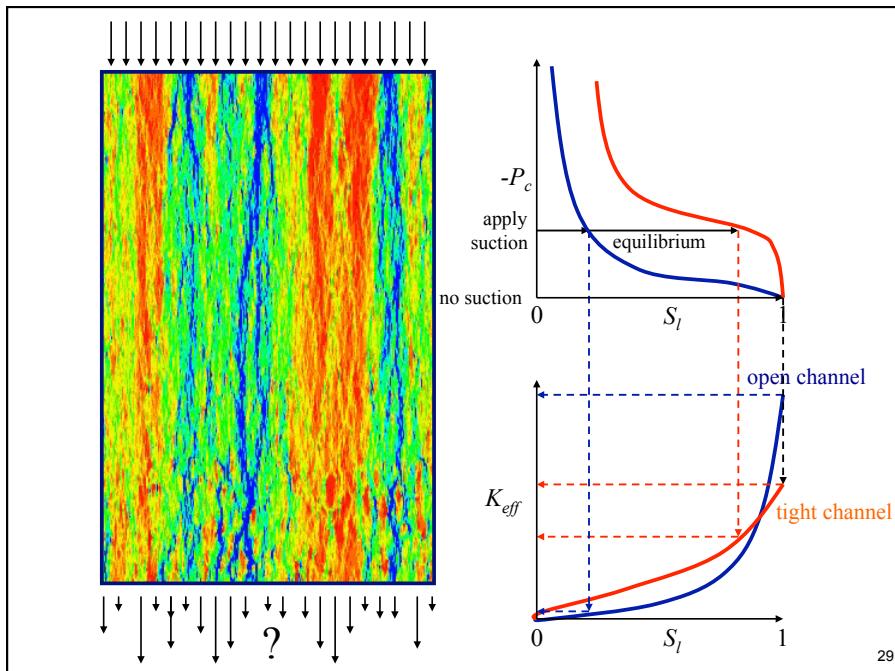


27

Fitting Laboratory Measurements of Relative Permeability



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Practice with Relative Permeability and Capillary Pressure Functions

- PetraSim spreadsheet for rel. perm. and cap. pres. functions *as implemented in TOUGH2*
 - <http://www.thunderheadeng.com>
 - Click on *PetraSim* link
 - Click on *Support Resources* link
 - Scroll down to *Tools*
- Click on [relative_permeabilities_V2.xls](#)
- Click on [capillary_pressure.xls](#)
- These spreadsheets can be downloaded for free
- When starting a new problem, try out the Pcap and RelPerm parameters in the spreadsheets

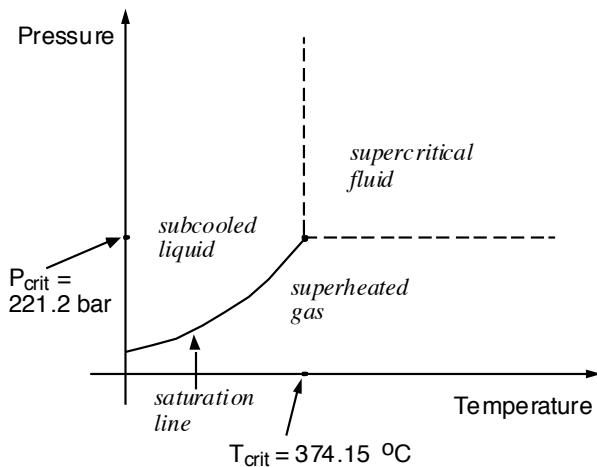
30

Equation Of State

- Fluid properties ... (secondary parameters)
 - Density
 - Viscosity
 - Internal energy
- ... as a function of state variables (primary variables)
 - Pressure
 - Temperature
 - Concentration
- *Link between primary variables and secondary parameters*
- Determines *phase state* and *phase composition*
- Different EOS modules to handle different fluids

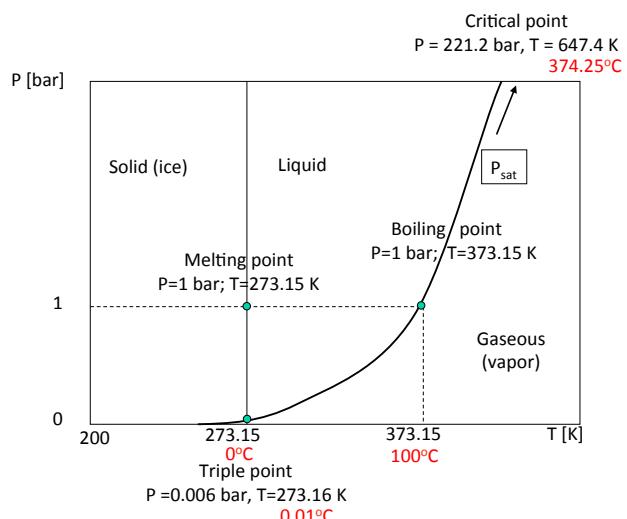
31

Phase Diagram for a Single-Component Water System

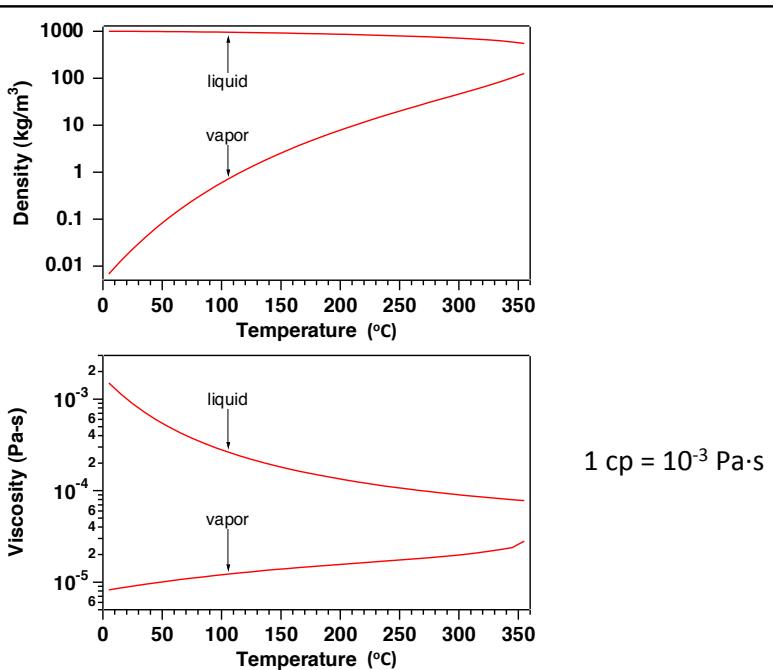


32

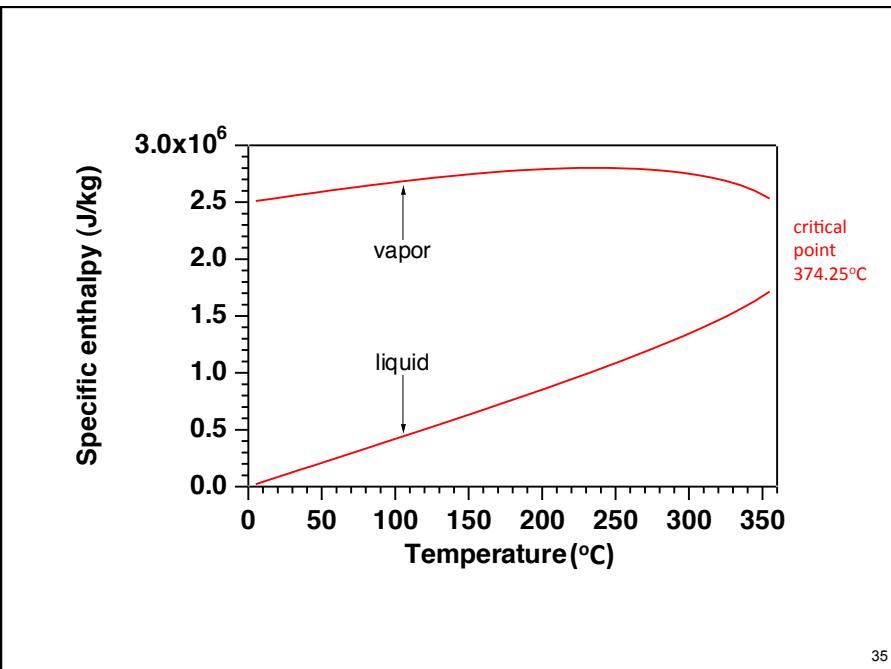
Vapor Pressure Curve for Water



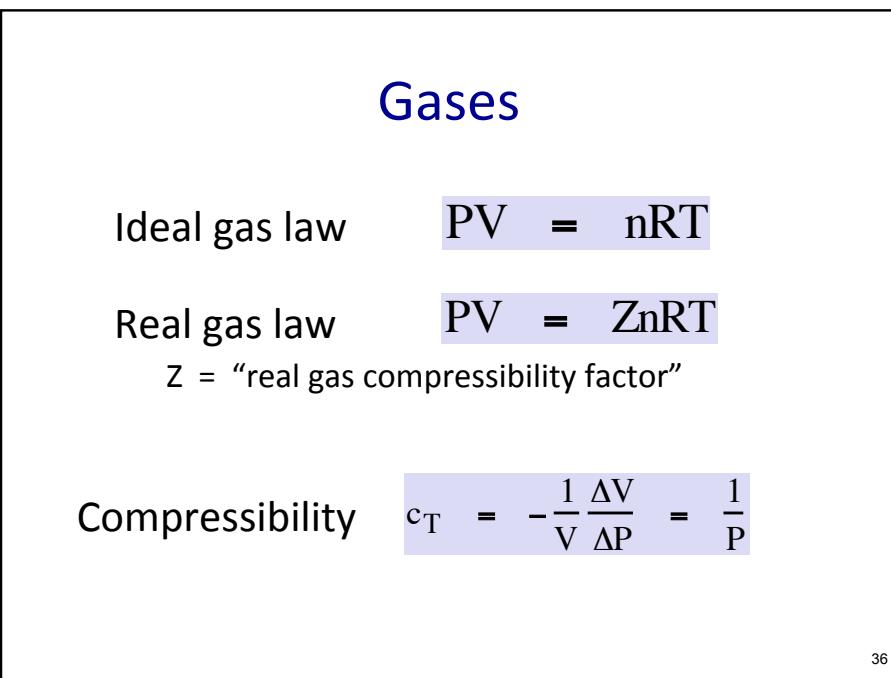
33



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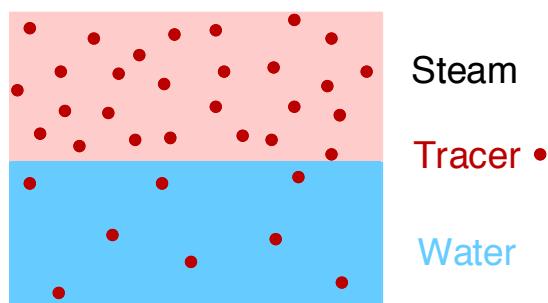


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Phase Partitioning

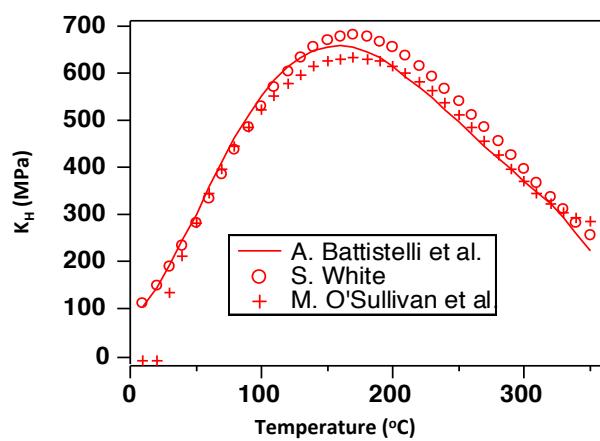
Henry's Law

$$P_{NCG} = K_h x_{aq}^{NCG}$$



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Henry's coefficient for dissolution of CO₂ in water



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Two-Component Systems

Dalton's Law: $P_{tot} = \sum_{\kappa=1}^{NK} P_g^\kappa$
(for ideal gases)

P_g^κ = vapor partial pressure of κ
in equilibrium with solution

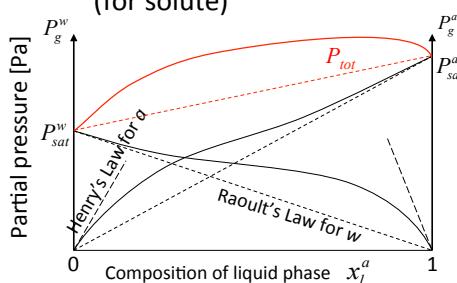
$$P_g^\kappa / P_g = n_g^\kappa / n_g = x_g^\kappa = \text{mole fraction in gas}$$

Raoult's Law: $P_g^\kappa = x_l^\kappa \cdot P_{sat}^\kappa$
(for solvent)

x_l^κ = mole fraction in solution

Henry's Law: $P_g^\kappa = h^\kappa \cdot x_l^\kappa$
(for solute)

h^κ = Henry's coefficient
[Pa/mole fraction]



TOUGH2 uses mass fraction instead of mole fraction

$$\begin{aligned} P_g^\kappa &= H^\kappa \cdot X_l^\kappa \\ H^a &\approx 10^{10} \text{ Pa} \\ H^{CO_2} &\approx 10^8 \text{ Pa} \end{aligned}$$

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Nonisothermal Flow: Heat Balance Equation

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Definitions

- T [K]: intensive state variable
- Heat [$\text{J} = \text{kg m}^2 \text{s}^{-2}$]: extensive state variable = ρcTV
- Internal energy U [J]: total energy of its molecules = $f(T)$
- Specific internal energy u [J kg^{-1}]
- Specific heat capacity c_v [$\text{J kg}^{-1} \text{K}^{-1}$]: $c_v = \partial u / \partial T$
energy needed to increase T of 1 kg by 1 K at constant volume
- Enthalpy $H = U + pV$ [J]: Sum of internal energy and energy needed to change volume (pV); energy available for mechanical work.
- Specific enthalpy [J kg^{-1}]: $h = u + p/\rho$
- Specific heat capacity for constant pressure: $c_p = \partial h / \partial T$
- Ideal gases: $c_p - c_v = R/M$ ($R = 8.314 \text{ [J mol}^{-1} \text{ K}^{-1}\text{]}$)
- Entropy: thermal energy not available for work; measure of randomness/disorder

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Heat Balance Equation

- Balance Equation for Heat [J s^{-1}]:

$$\frac{d}{dt} \int_{V_h} M^h dV_n = \int_{\Gamma_n} \mathbf{F}^h \cdot \mathbf{n} d\Gamma_n + \int_{V_h} q^h dV_n$$

- Specific Heat [J m^{-3}]:

$$M^h = (1 - \phi) \rho_R \cdot c_R \cdot T + \phi \sum_{\beta} S_{\beta} \cdot \rho_{\beta} \cdot u_{\beta}$$

- Specific Heat Flux [$\text{J m}^{-2} \text{s}^{-1}$]:

$$\mathbf{F}^h = -\lambda \nabla T + \sum_{\beta} h_{\beta} \cdot \mathbf{F}_{\beta}$$

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Thermal Properties

- Heat conductivity λ $[J \text{ s}^{-1} \text{ m}^{-1} \text{ K}^{-1}]$
- Specific heat c $[J \text{ kg}^{-1} \text{ K}^{-1}]$
- Thermal expansivity $\frac{1}{\phi} \frac{\partial \phi}{\partial T} \Big|_p$ $[K^{-1}]$
- Volumetric heat capacity $C = \rho c$ $[J \text{ m}^{-3} \text{ K}^{-1}]$
- Thermal diffusivity $D_T = \frac{\lambda}{\rho c}$ $[m^2 \text{ s}^{-1}]$
- Radiant emittance ε [-]

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Multiphase Thermal Properties

- **Heat capacity**
 - Internal energy of fluid phases provided by EOS module
 - Provide specific heat and rock grain density for solid phase
 - TOUGH calculates volume-weighted average
- **Thermal conductivity**
 - Depends on conductivities of solid and fluid phases
 - Depends on geometry of phase connectivity
 - Requires empirical relationship $\lambda = \lambda(S)$
 - Specify effective wet and dry thermal conductivities
 - See MOP (10) for choices

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Heat Conductivity and Specific Heat

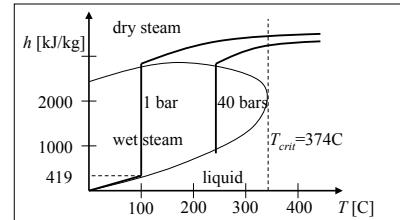
Medium	λ [W m ⁻¹ K ⁻¹]	$C=\rho c$ [kJ m ⁻³ K ⁻¹]
Air	0.026	1.25
Water (l)	0.598	4180
Ice	2.2	1900
Silver	427	
Iron	81	
Salt	5.9	
Quartz	6	~2000
Granite	2.5-3.8	~2000
Dry sand	0.4-0.8	
Wet sand	2.5-3.5	
Dry clay	0.8-2.0	
Wet clay	1.2-1.7	
Sandstone	1.5-4.3	

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Latent Heat

- Latent heat/heat of transformation:
 - Heat of fusion/vaporization/sublimation
 - no change in temperature
- Evaporation: heat-absorbing (endothermic)
- Condensation: heat-releasing (exothermic)
- Difference between enthalpy of liquid water (419 kJ/kg) and pure steam (2677 kJ/kg) = 2258 kJ/kg

- Heat pipe



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Other Processes

- Radionuclide transport
- Adsorption
- Multiphase binary diffusion
- Klinkenberg effect
- Vapor pressure lowering

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Radionuclide Transport

- Radionuclide Decay:
 - Parent radionuclide:
 - Daughter radionuclide:
- Half Life:
- Parent-Daughter Decay Chain Examples:
 - Radioactive Decay: $^{234}\text{U} \rightarrow ^{230}\text{Th} \rightarrow ^{226}\text{Ra}$
 - Dechlorination: PCE \rightarrow TCE \rightarrow DCE \rightarrow VC \rightarrow ETH
 - Nitrification: ammonium (NH_4^+) \rightarrow nitrite (NO_2^-) \rightarrow nitrate (NO_3^-)

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More Processes

- Linear Equilibrium Adsorption:

$$M^\kappa = \phi \sum_\beta S_\beta \rho_\beta X_\beta^\kappa + (1 - \phi) \rho_R \rho_{aq} X_{aq}^\kappa K_d^\kappa$$

- Multiphase Diffusion:

$$\mathbf{f}^\kappa = - \sum_\beta \varphi \tau_0 \tau_\beta \rho_\beta d_\beta^\kappa \nabla X_\beta^\kappa$$

- Klinkenberg Effect:

$$k_g = k_l \left(1 + \frac{b}{P_g} \right)$$

- Vapor Pressure Lowering: $P_v(T, S_i) = f_{VPL}(T, S_i) \cdot P_{\text{sat}}(T)$

$$f_{VPL} = \exp \left[\frac{M_w P_c(S_l)}{\rho_l R (T + 273.15)} \right]$$

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TOUGH Overview

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Outline

- Overview of capabilities
- Architecture
- Input
 - General concept
 - Main input blocks
 - Format
 - Files

2

1

That's TOUGH!

TOUGH: Transport Of Unsaturated Groundwater and Heat

multidimensional	0D, 1D, 2D, 3D
multiphase	liquid, gas, NAPL
multicomponent	water, air, VOC, radionuclides
nonisothermal	heat
flow and transport	multiphase Darcy law
fractured-porous media	DFN, dual- ϕ , dual-k, MINC, ECM

EOS: Equation-Of-State

Accurate description of thermophysical properties

3

TOUGH Summary

- **multiphase flow**
 - pressure, viscous, gravitational forces
 - capillary pressure, relative permeability
 - vapor pressure lowering
 - appearance/disappearance of phases
 - accurate thermodynamic properties
- **multicomponent**
 - phase partitioning, dissolution/precipitation
 - sorption, multiphase diffusion
 - parent-daughter decay of radionuclides

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TOUGH Summary (cont.)

- **nonisothermal**
 - heat convection/conduction/diffusion
 - latent heat effects (evaporation/condensation)
 - radiative heat transfer
 - semi-analytical heat exchange with confining layers and wells
- **fractured-porous media**
 - discrete fracture network
 - equivalent continuum model
 - double-porosity
 - dual-permeability
 - multiple interacting continua (MINC)

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TOUGH Summary (cont.)

- Integral Finite Differences
- Fully coupled (mass and energy)
- Fully implicit
- Permeability/mobility weighting options
- Newton-Raphson
- Absolute and relative residual convergence criteria
- Direct and iterative linear equation solvers

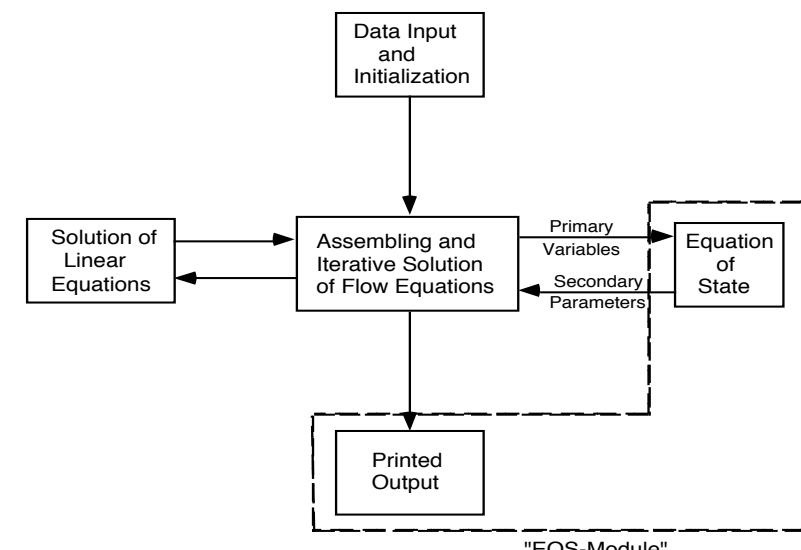
6

Architecture

- Balance equations for multiphase, multicomponent and heat flow have identical mathematical form, regardless of number of and nature of components and phases.
- Differences in fluid systems (types of components and phases present) is only in fluid properties.
- “Modular” architecture:
 - Core module for assembling flow and transport equation
 - Equation-of-state (EOS) module: thermophysical and transport properties
 - Module for linear equation solver
 - Modules for input/output

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Modular Architecture for TOUGH2



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Equation-of-State Modules

- EOS1 : water, tracer, heat
- EOS2 : water, CO₂, heat
- EOS3 : water, air, heat
- EOS4 : water, air, heat, VPL
- EOS5 : water, hydrogen, heat
- EOS7 : water, brine, air, heat
- EOS7r : water, brine, RN1, RN2, air, heat
- EOS8 : water, oil, NCG, heat
- EOS9 : water (variably unsaturated: Richards' equation)
- EWASG : water, brine, NCG, heat
- ECO2N : water, brine, CO₂, heat
- ECO2M : water, brine, CO₂, heat (multiphase)
- T2VOC : water, air, VOC, heat
- TMVOC : water, air, m VOCs, m NCGs, heat

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Additional Modules/Packages

EOS7C	: H ₂ O, CO ₂ /N ₂ , CH ₄ , tracer, heat
TOUGHREACT	: Reactive transport
GoldSim-TOUGH	: System-level modeling
iTOUGH2	: Inverse modeling
iTOUGH2-geophysics	: Add geophysical data
TOUGH-CLM3	: Land-surface model
TOUGH-FLAC	: Geomechanics
TOUGH2-MP	: Parallelization
TOUGH+Hydrate	: Gas hydrates
T2Well	: Wellbore-reservoir simulator

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Formatted Text Input

- No graphical user interface is part of TOUGH2 (check Pre- Postprocessing tab at <http://esd.lbl.gov/TOUGH>)
- Text-based (ASCII) input file → use text editor (e.g., TextPad, WordPad, Notepad, EDIT, ..., without saving formatting characters), and *without using tabs*
- Input file has *strict formatting* requirements → see FORTRAN formatting statements in manual, e.g.:

Format (**A5, 5X, 2E10.4**)

- Columns 1-5: **5-character string**
- Columns 6-10: **5 spaces**
- Columns 11-20, 21-30: **Two real numbers**
max. 10 digits
format irrelevant
include decimal point

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Main Input Blocks

- 5-character *keywords* in columns 1-5 indicate main input blocks:
 - Mesh: MESHM, ELEME, CONNE
 - Material properties: ROCKS, RPCAP, SELEC, DIFFU
 - Initial/boundary conditions: INDOM, INCON, GENER
 - Computational parameters: PARAM, SOLVR, MULTI, ENDCY
 - Output: TIMES, FOFT, COFT, GOFT
- Certain blocks can be provided in *external files*:
 - *MESH, INCON, GENER*
- Blocks of variable length (ROCKS, ELEME, CONNE, GENER, INCON, INDOM) need to be terminated by an *empty line*

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TOUGH2 Input Format

TOUGH2 INPUT FORMATS											
TITLE											
ROCKS	1	*	2	3	4	*	5	*	6	7	*
MAT	NAD	DROK	POR	PER (1)	PER (2)	PER (3)	CWET	SPHT			
COM		EXPAN	CDRY	TORTX	GK	XKD3	XKD4				
IRP		RP (1)	RP (2)	RP (3)	RP (4)	RP (5)	RP (6)	RP (7)			
ICP		CP (1)	CP (2)	CP (3)	CP (4)	CP (5)	CP (6)	CP (7)			
MULTI	(optional)	*	2	*	3	*	4	*	5	*	6
NK	NEQ	NPH	NB	NKIN							
START	(optional)	*	2	*	3	*	4	*	5	*	6
MOP:	1	2	3	4	5	6	7	8	9	10	11
MOP:	1	2	3	4	5	6	7	8	9	10	11
PARAM	1	*	2	*	3	*	4	*	5	*	6
NCYC	MSEC	MCYPR	MOP (4), I=1,24				TEXP	BE			
TSTART		TIMEA	DELTEN or NDLT	DELMX	ELST		GF		REDUT	SCALE	
DLT (1)	DLT (2)	DLT (3)						DLT (4)	(M\$B*NDLT)		
RE1	RE2	U	WUJP	WNR	DFAC						
DEP (1)	DEP (2)	DEP (3)	DEP (4)								
SOLVR	(optional)	*	2	*	3	*	4	*	5	*	6
ZPROCS		RITMAX	CLOSUR								
RPCAP	(optional)	*	2	*	3	*	4	*	5	*	6
IRP		RP (1)	RP (2)	RP (3)	RP (4)	RP (5)	RP (6)	RP (7)			
ICP		CP (1)	CP (2)	CP (3)	CP (4)	CP (5)	CP (6)	CP (7)			

see Manual p. 22-24

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TOUGH2 Input Format (cont'd)

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TOUGH2 Input Format (cont'd)

SELEC (optional)															
IE(1)	IE(2)	IE(3)	IE(4)	IE(5)	IE(6)	IE(7)	IE(8)	IE(9)	IE(10)	IE(11)	IE(12)	IE(13)	IE(14)	IE(15)	IE(16)
FE(1)	FE(2)	FE(3)	FE(4)	FE(5)	FE(6)	FE(7)	FE(8)	FE(9)	FE(10)	FE(11)	FE(12)	FE(13)	FE(14)	FE(15)	FE(16)
FE(17)															
															FE18*IE(1)
TIMES (optional)															
ITI	ITE	DELAY	TINTER												
TIS (1)	TIS (2)	TIS (3)													TIS (ITI)
MESHM (optional)															
FOFT (optional)															
EOFT															
COFT (optional)															
ECOFT															
GOFT (optional)															
EGOFT															
NOVER (optional)															
ENDFI															
ENDCY															

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General Remarks

- Blank space may invoke (non-zero!) **default** value!
- Many **hidden flags**; examples:
 - SPHT
 - non-zero/negative values
 - special domain names (REFCO, SEED)
- Some blocks are optional
- Blocks can be provided in (*almost*) any order; exceptions:
 - First line must be title line
 - ELEME before CONNE
 - START before INCON
 - MULTI before PARAM, INDOM, and INCON (**only if NKIN≠NK**)
 - Follow convention (suggestion: TITLE, ROCKS, RPCAP, PARAM, ELEME, CONNE, GENER, INCON, ENDCY)

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Files

- Main input file (arbitrary name + *.txt or blank*)
- Optional input files:
 - *MESH*: Grid (blocks `ELEME` and `CONNE`)
 - *INCON*: Initial conditions
 - *GENER*: Neumann boundary conditions
- Main output file (arbitrary name + *.out*)
- Additional output files
 - *SAVE*: final system state (set of primary variables)
→ initial conditions for continuation run
 - *LINEQ, VERS*
 - *TABLE, FOFT, COFT, GOFT*
 - *MESH, MINC, INCON, GENER*

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Output

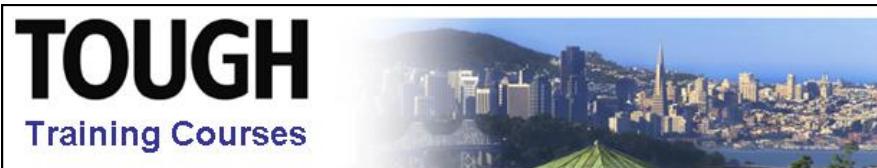
- No graphical output
- Some postprocessors available, check:
[http://esd.lbl.gov/research/projects/tough/
software/processors.html](http://esd.lbl.gov/research/projects/tough/software/processors.html)
- Main ASCII output file
- Special output files

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Got Bugs?

- Users have to assume that the code has bugs - it is the user's responsibility to check and verify their code applications.
- What to do?
 - be very careful in writing/changing codes and developing applications
 - keep unbroken chain of test applications and sample problems
 - compare with semi-analytical solutions, other codes
 - compare with data (lab, field)
 - maintain records (internal version control)
 - wide dissemination: the more a code gets used, the greater the likelihood that bugs will be found and fixed
 - inform developers
 - user forum (<http://tough.forumbee.com/>)

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Code Installation

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Compiling Source Code

- Source code for TOUGH2 v2.1 consists of FORTRAN files, such as *t2cg22.f*, *meshm.f*, *t2f.f*, *t2fm.f*, *t2solv.f*, and *eosX.f* (one of the equation-of-state modules)
- Dimension major arrays in file *T2*
- May need to adjust machine-dependent subroutines (e.g., CPU-time)
- May need to rename duplicate subroutines (see *read.me* file)
- Compile source files to create EOS-specific executable (e.g., *xt2_eosX.exe*) that links core and EOS module (*eosX.o*)

2

Excerpt from T2

```

*****
C***** file 'T2' for module t2cg22.f of TOUGH2, Version 2.1 *****
C*****
C*
C*      ASSIGN PARAMETERS FOR FLEXIBLE DIMENSIONING OF LARGE ARRAYS *
C*
C*****
C
C
C      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
C
C
C
C--- MNEL: Number of elements
C         PARAMETER (MNEL = 12000)
C
C--- MNCON: Number of connections
C         PARAMETER (MNCON = 25000)
C
C--- MNEQ: Number of equations per element (# of Primary variables)
C         PARAMETER (MNEQ = 4)
C
C--- MNK: Number of components
C         PARAMETER (MNK = 3)
C
C--- MNPH: Number of phases which can be present
C         PARAMETER (MNPH = 3)
C
C--- MNB: Number of phase-dependent secondary variables
C         PARAMETER (MNB = 8)
...

```

3

Installation for Short Course on PC

- Executables are provided for this short course
 - ***Obtain your own TOUGH2 license!***
1. Copy course material folder from flash drive to a new directory on your hard drive, e.g., C:\TOUGH2
 2. Two options:
 - 2a. Copy the relevant executable to the directory where your input files are (needs to be done for each working directory), or...
 - 2b. ...add C:\TOUGH2\Executables\PC
to the command search path (needs to be done only once):
 - START → Settings → Control Panel → System → Advanced → Environment Variables
 - Edit “Path” under System variables
 - Add semi-colon and path name at the end of “Variable value”:
; C:\TOUGH2\Executables\PC

Running TOUGH on PC

- Open a DOS Command Window:
 - START → Run... → type: cmd
- Change to working directory, e.g.:


```
cd C:\TOUGH2\Exercises\Problem_Tutorial
```
- Two options:
 1. Copy relevant TOUGH2 executable, e.g., for EOS3 copy file
C:\TOUGH2\Executables\PC\t2_eos3.exe
to working directory, e.g., to
C:\TOUGH2\Exercises\Problem_Tutorial
 2. Add directory holding the executable to command search path (see previous slide; needs to be done only once).
- Run TOUGH2 from the command line in the DOS Window, redirecting standard input (<) and standard output (>), e.g.:


```
xt2_eos3.exe < Pla.txt > Pla.out.txt
```

Installation for Short Course on MAC

- Executables are provided for this short course
- ***Obtain your own TOUGH2 license!***
- Copy course material folder from flash drive to a new directory \$HOME/TOUGH2 on your hard drive
- Copy the relevant executable to the directory where your input files are, or...
- ...add \$HOME/TOUGH2/Executables/MAC
to the command search path (for bash shell):
 - open a Terminal (
 - edit file `~/.bashrc` and add the following line:
`PATH=$PATH:$HOME/TOUGH2/Executables/MAC`
 - save file and quite editor
 - type:
`source ~/.bashrc`

Running TOUGH on MAC

- Open a Terminal (█):
- Change to the working directory, e.g.:
`cd ~/TOUGH2/Exercises/Problem_Tutorial`
- Run TOUGH2 from command line in Terminal, redirecting standard input (<) and standard output (>), e.g.:
`xt2_eos3.mac < Pla.txt > Pla.out`
- If you copied the executable to the working directory rather than defining the command search path in file `~/.bashrc` (see previous slide), you may need to add `./`, i.e.:
`./xt2_eos3.mac < Pla.txt > Pla.out`

Useful Programs

- Textpad for text editing, file comparison:
<http://www.textpad.com/download/>
- Relative permeability and capillary pressure curves (under Tools):
<http://www.thunderheadeng.com/petrasim/petrasim-resources/#target5>
- Steam table:
<http://www.steamtablesonline.com/steam97web.aspx>
- Thermodynamic properties:
<http://webbook.nist.gov/chemistry/>
- Other TOUGH related free software:
<http://esd.lbl.gov/research/projects/tough/licensing/free.html>



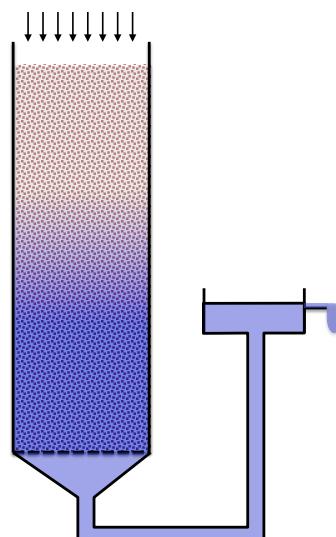
Building a TOUGH2 Model Step by Step

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Problem Statement

- Column experiment
- Filled with homogeneous sand
- Initially fully saturated
- Simulate experiments:
 1. Establish **hydrostatic** initial conditions
 2. **Drain** column, establishing a water table 1/3 from the bottom and creating an unsaturated zone in the upper part of the column
 3. **Explore** other potential experimental phases or properties



2

1

Step by Step...

- Rock Properties
- Mesh Generation
- Initial and Boundary Conditions
- Computational Parameters

3



Material Properties

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

4

2

Outline Material Properties

- General Concept
- Block **ROCKS**
- Block **RPCAP**
- Additional blocks with properties
- Exercise 1a

5

Material Properties

- General approach
 - Subdivide model domain into zones of equal properties (zonation approach)
 - Specify material name (in block **ROCKS**)
 - Specify material properties (hydrological, thermal; in block **ROCKS**)
 - Associate each element with a material name (in block **ELEM**)
 - (Element-by-element permeabilities and porosities possible; see special material **SEED**; variable **PMX** in block **ELEM**, and block **INCON**)
- TOUGH input blocks
 - **ROCKS**: Hydrological and thermal properties
 - **RPCAP**: Default relative permeability and capillary pressure curves
- Fluid properties
 - Provided *internally*, i.e., no input required; see fluid-specific EOS modules
 - Exceptions:
 - Certain VOC and brine properties (block **SELEC**, **DIFFU**)
 - Reference properties for water in EOS9 (special “material” **REFCO**)
- Properties of boundary elements
 - Pay special attention to properties of boundary elements, e.g., atmospheric boundary
<http://esd.lbl.gov/files/research/projects/tough/support/atmo-boundary-condition.pdf>

6

Block ROCKS

- Material name (5-character, case-sensitive)
- Hydrological properties
 - Porosity
 - Absolute permeability [m^2] in three (arbitrary) directions (see variable ISOT in block CONNE)
 - Parameters of relative permeability and capillary pressure functions (overwrite defaults given in block RPCAP)
- Thermal properties
 - Rock grain density [kg/m^3]
 - Formation heat conductivity (wet) [$\text{W}/\text{m}^\circ\text{C}$]
 - Rock grain specific heat [$\text{J}/\text{kg}^\circ\text{C}$] (mass balance flag if $>1\text{E}4$)

Name	NAD	DROK	PORO	PER (1)	PER (2)	PER (3)	CWET	SPHT
ROCKS	1	*	2	*	3	*	4	*
SAND	0	2650.	.4000	1.000E-12	1.000E-12	1.000E-13	2.51	920.
GRAVE	0	2650.	.3000	1.000E-11	1.000E-11	1.000E-11	2.51	920.
BOUND	0	2650.	.9900	1.000E-12	1.000E-12	1.000E-12	2.51	10000.
(empty line closes ROCKS block)								

Block ROCKS with NAD > 0

- If NAD = 1, read *one* additional line
 - Pore compressibility [Pa^{-1}]
 - Pore expansivity [$^\circ\text{C}^{-1}$]
 - Dry thermal conductivity [$\text{W}/\text{m}^\circ\text{C}$] (see also MOP (10))
 - Tortuosity parameter (for diffusion; see Appendix D.4)
 - Klinkenberg parameter, b [Pa^{-1}], $k_{\text{gas}} = k_{\text{abs}}(1 + b/P)$
 - Adsorption coefficients, K_d [kg m^{-3}] (EOS7r only)
- If NAD = 2, read *three* additional lines
 - first line: see NAD = 1
 - second line: parameters of relative permeability curves
 - third line: parameters of capillary pressure curve
(second and third line have same format as block RPCAP)

COM	EXAN	CDRY	TORTX	GK	XKD3	XKD4
ROCKS	1	*	2	*	3	*
SHALE	2	2650.	.1200	1.000E-18	1.000E-18	1.000E-20
	1.0E-09	1.0E-05	1.5	0.0	1.0E+06	2.51 800.
	3	0.3	0.1			
	1	1.0E7	0.0	1.0		

Block RPCAP

- Default relative permeability and capillary pressure functions, assigned to all materials with NAD≤1
- Overwritten by ROCKS .3 and ROCKS .4 if NAD = 2
- First line: Relative permeability function
- Second line: Capillary pressure function
- Select **type of curve** by number
- Provide curve-specific **parameters**
- See TOUGH2 manual, Appendices G and H

```
RPCAP----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
      3          0.3      0.1
      1          0.0      0.0      1.0
```

9

Characteristic Curves

- van Genuchten-Mualem relative permeability functions (\sim IRP=7)

$$k_{rl} = S_e^\varepsilon \left[1 - \left(1 - S_e^{1/m} \right)^m \right]^2$$
$$k_{rg} = (1 - S_e)^\gamma \left[1 - S_e^{1/m} \right]^{2m}$$

- van Genuchten capillary-pressure function (\sim ICP=7)

$$p_c = -\frac{1}{\alpha} \left[S_e^{-1/m} - 1 \right]^{1/n}$$

- Code your own rel. perm. and cap. pres. functions into subroutines RELP and PCAP, respectively

10

Additional Properties

- Additional, EOS-specific fluid properties and other parameters are given in blocks SELEC and DIFFU (see Manual)
- For EOS9 (Richards equation):
 - Reference water properties given in special “domain” REFCO.

```
ROCKS----1-----2-----3-----4-----5-----6-----7-----8
SAND      2650.    .4000 1.000E-12 1.000E-12 1.000E-13     2.51     920.
REFCO     1.013E05   15.0   999.213 1.135E-03 4.594E-10

Special name  Press.    Temp.    Density Viscosity Compressibility
```

11

Assign Properties to Elements

- In block ELEME, assign domain by
 - Name, or
 - Sequence number in block ROCKS
- In block CONNE, provide 1, 2, or 3 (ISOT) to indicate (anisotropic) permeability (PER (ISOT))

```
ELEME
A11 1      BOUND 0.1000E-090.1000E+01      0.5000E+000.5000E+00-.5000E-10
A21 1      SAND  0.5000E-010.0000E+00      0.5000E+000.5000E+00-.2500E-01
A31 1      30.5000E-010.0000E+00      0.5000E+000.5000E+00-.7500E-01
A41 1      30.5000E-010.0000E+00      0.5000E+000.5000E+00-.1250E+00

CONNE
A11 1A21 1      10.5000E-100.2500E-010.1000E+01
A21 1A31 1      20.2500E-010.2500E-010.1000E+01
A31 1A41 1      30.2500E-010.2500E-010.1000E+010.1000E+01
```

ISOT

12

TOUGH

Training Courses



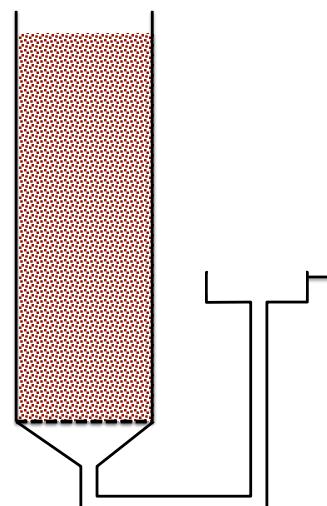
Exercise 1a

- Rock Properties
- Mesh Generation
- Initial and Boundary Conditions
- Computational Parameters

13

Exercise 1a: Material Properties

- Assume column is filled with *homogeneous* sand
- Identify hydrological properties of sand
- Identify properties for boundary elements
- Create blocks ROCKS and RPCAP



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Conceptual Model

Q1: Describe the conceptual model (i.e., what assumptions do you make when abstracting the real system to create a model?)

Q2: Pick appropriate equation-of-state module

15

Question ROCKS

Q3: Identify the (minimum) parameter set needed to run Sample 1, and collect appropriate parameter values for a clean sand.

16

Question RPCAP

Q4: Select the *van Genuchten* [1980] relative permeability and capillary pressure functions, and define appropriate parameter values (see Appendices G and H)

17

Blocks ROCKS and RPCAP

- Open file *P1a.txt* and fill in blocks ROCKS and RPCAP

Note: Remember to terminate block `ROCKS` with an empty line (does block `RPCAP` need an empty line?)

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Questions REFCO

Q5: A special domain REFCO (EOS9 only!) is available in block ROCKS. Discuss its parameters.

Q6: What would happen if you assigned (a) a value of zero, and (b) a value of 1E-99 to parameter PER (3) in REFCO?

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Numerical Method

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Outline

- Integral finite difference method
- Space discretization
- Time discretization

2

1

Integral Finite Difference Method

- In the **Integral Finite Difference** (IFD) method, space discretization is made directly from the integral equations:

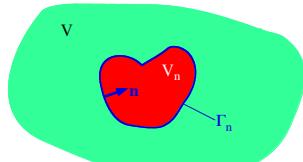
$$\frac{d}{dt} \int_{V_n} M^\kappa dV_n = \oint_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^\kappa dV_n$$

(i.e., no PDE is derived and then integrated)

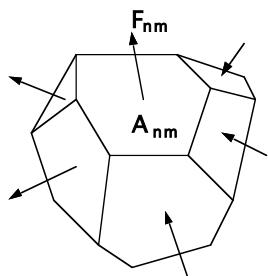
3

Integral Finite Differences (IFD)

replace integrals with averaged mass densities
and discrete sums of average mass fluxes



$$\int_{V_n} M dV = V_n M_n$$



$$\oint_{\Gamma_n} \mathbf{F} \cdot \mathbf{n} d\Gamma = \sum_m A_{nm} F_{nm}$$

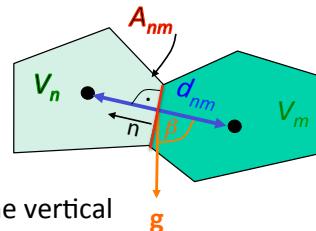
$$\frac{dM_n^\kappa}{dt} = \frac{1}{V_n} \sum_m A_{nm} F_{nm}^\kappa + q_n^\kappa$$

4

2

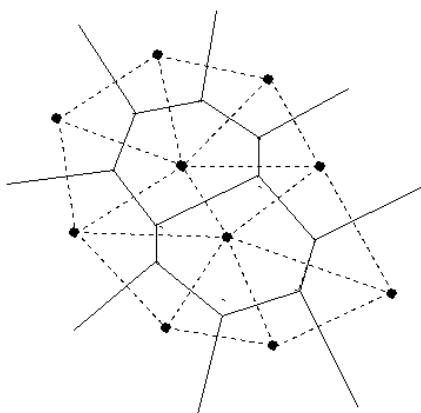
Space Discretization with IFD

- The system geometry is defined by:
 - volumes V of grid block
 - interface area A between grid blocks
 - nodal distances $d_{nm} = d_n + d_m$
 - orientation $\cos(\beta)$ of the nodal line to the vertical
- Orthogonality requirement: Line connecting two elements must be perpendicular to the interface
- The IFD does *not make reference to a global coordinate system*
- The IFD does not distinguish between 1-D, 2-D or 3-D systems; it combines *locally 1-D* subsystems
- Great flexibility in dealing with irregular geometries

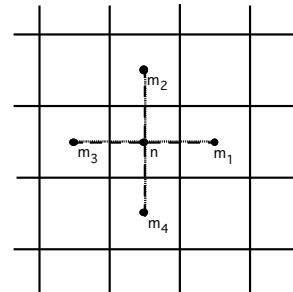


5

Orthogonality Requirement: Voronoi Tesselation

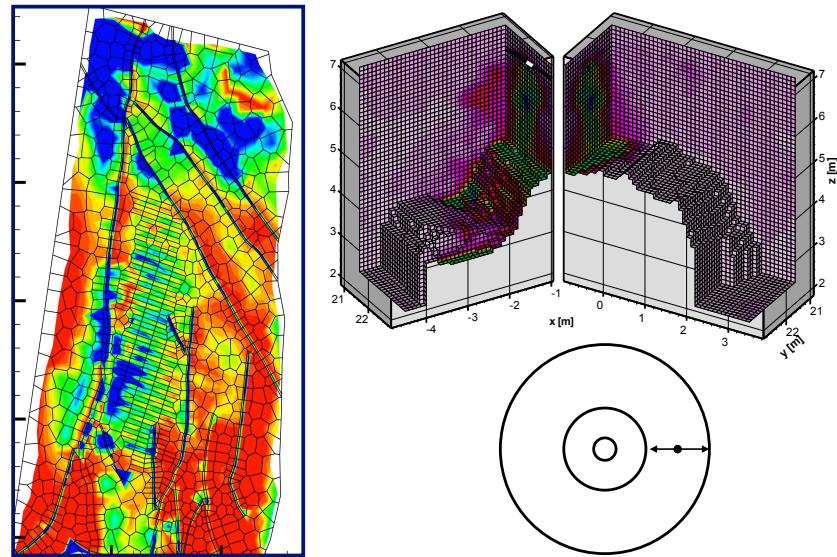


- start with arbitrary nodal points
- draw nodal lines (dashed)
- draw perpendicular bisectors
- partition plane into polygons (Voronoi tesselation)

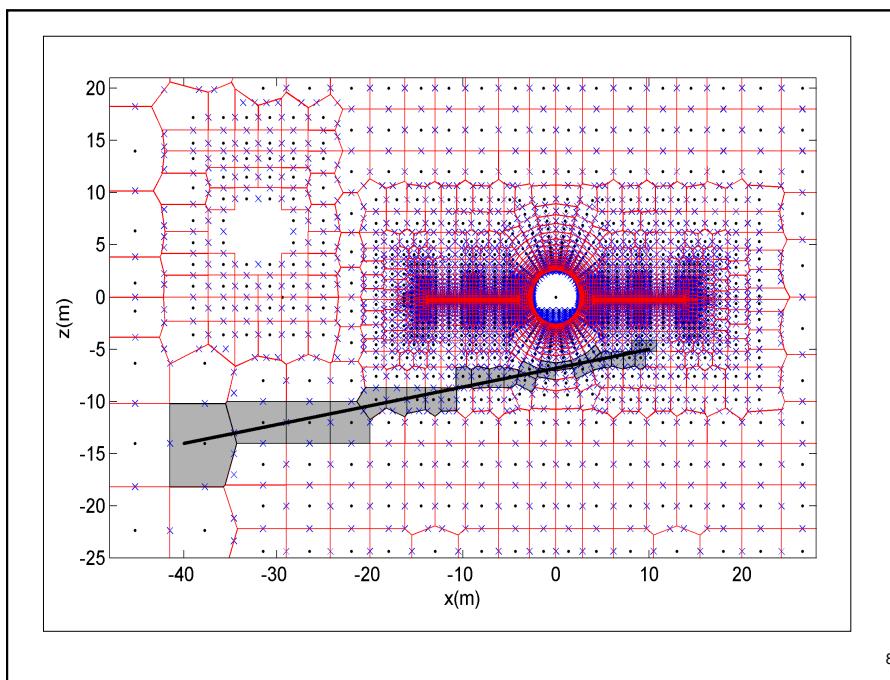


6

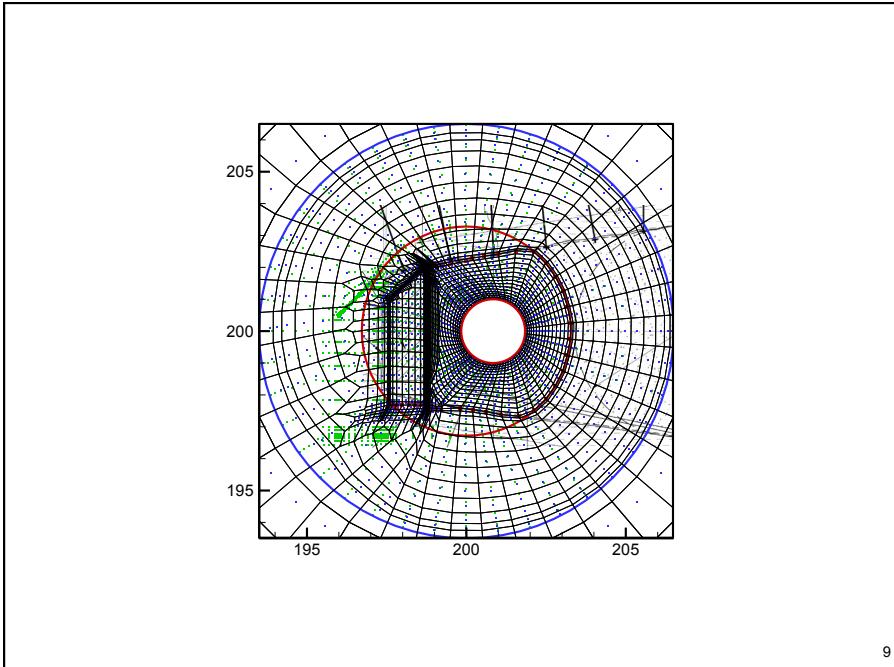
Voronoi Grids



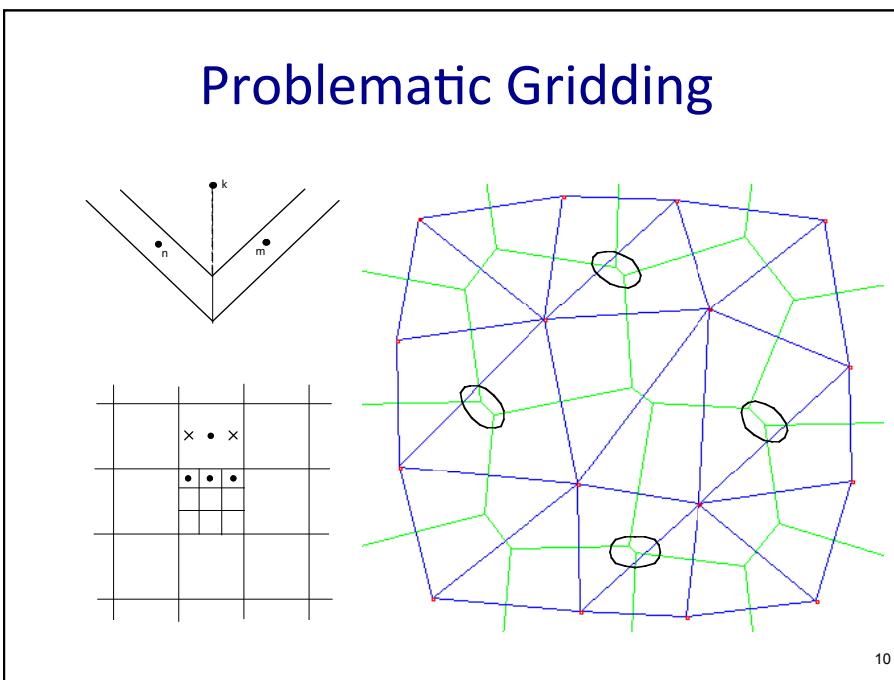
7



8

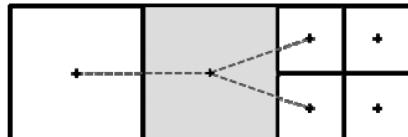


9

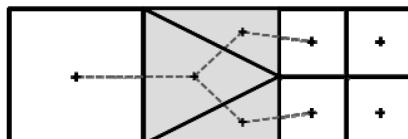


10

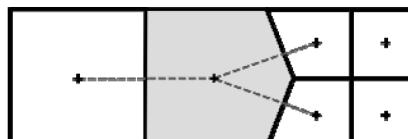
grid refinement



simple



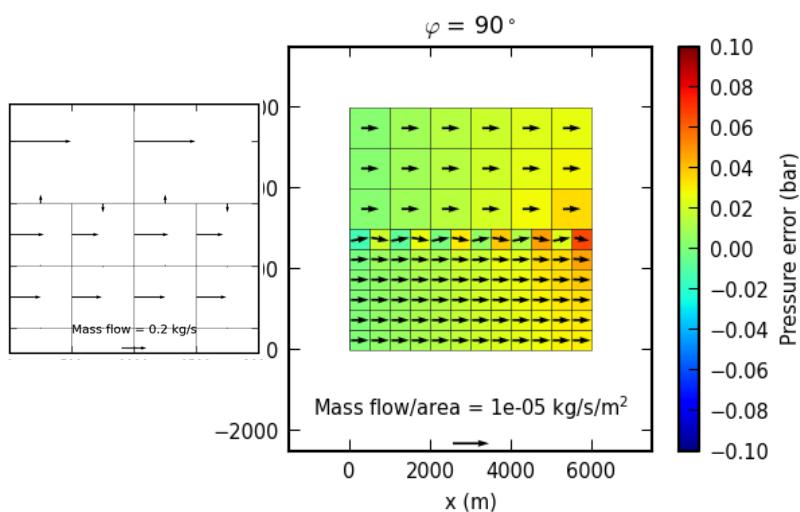
triangular



Voronoi

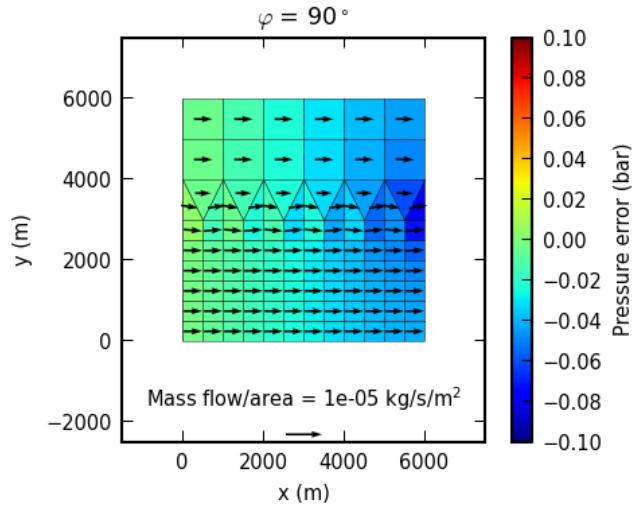
courtesy of Adrian Croucher 11

grid-orientation effects



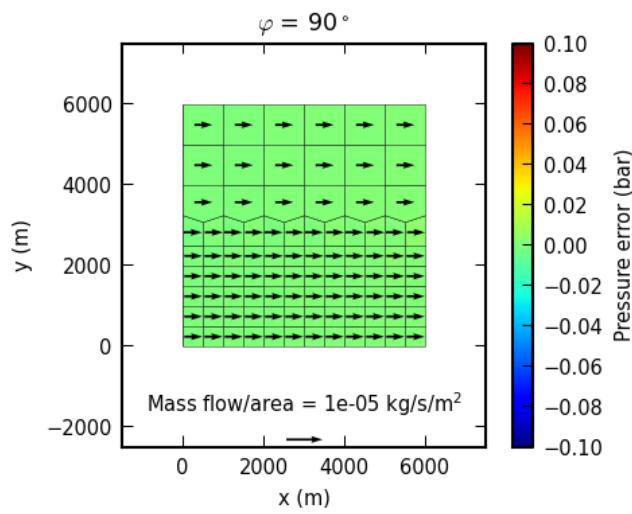
courtesy of Adrian Croucher 12

grid-orientation effects



courtesy of Adrian Croucher 13

grid-orientation effects



courtesy of Adrian Croucher 14

Grid Orientation Effects

rows	columns	1	2	3	4	5	6	7	8
1	
2	
3	
4	
5	
6	

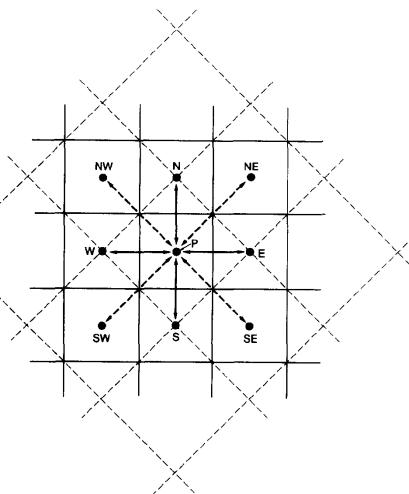
parallel grid

rows	columns	1	2	3	4	5	6	7	8	9	10	11
1	
2	
3	
4	
5	
6	
7	
8	
9	

diagonal grid

15

Five- and Nine-Point Finite Difference Approximations



16

Words to the Wise on Gridding

- When running simulations for field problems, where site-specific features should be modeled, *much of the work ends up dealing with geometry* (gridding).
- Meshes with many grid blocks make simulations run (much) more slowly, generate larger data files, and make it harder to understand what is going on.
- **Start with a simple, coarse grid**, and “debug” the problem.
 - facilitates data preparation
 - runs more easily and faster
 - smaller input and output files
 - makes it easier to understand what's happening
 - facilitates checking and debugging
- Put most problem features in place.
- After model is running satisfactorily, proceed to desired gridding and grid resolution.
- Check on grid sensitivity (“grid convergence study”).

17



Mesh Generation

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Step 2: Mesh Generation

- General Concept
- Element Information (block **ELEME**)
- Connection Information (block **CONNE**)
- Sample Problem 1b:
 - Mesh generation using MESHMAKER (block **MESHM**)

2

1

Mesh Generation

- General comments:

- Mesh generation is often the most tedious task
- Affects *efficiency, accuracy, robustness* of simulation
- Simple meshes: use internal mesh generator **MESHPACK** (Cartesian: XYZ, radial: RZ2D)
- Complex meshes: use external mesh generators (e.g., **PetraSim**, **WinGridder**, **AMESH**, **mView**, **TOUGH2GIS**, etc.)
- Almost always needs *manual modifications!*

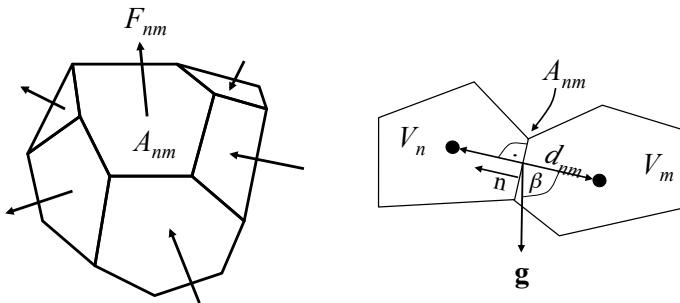
- Mesh design considerations:

- Minimize model domain (exploit symmetry)
- Minimize dimensionality
- Accommodate heterogeneity
- Anticipate steep gradients
- IFD: Dirichlet boundary conditions require specifying special boundary elements

3

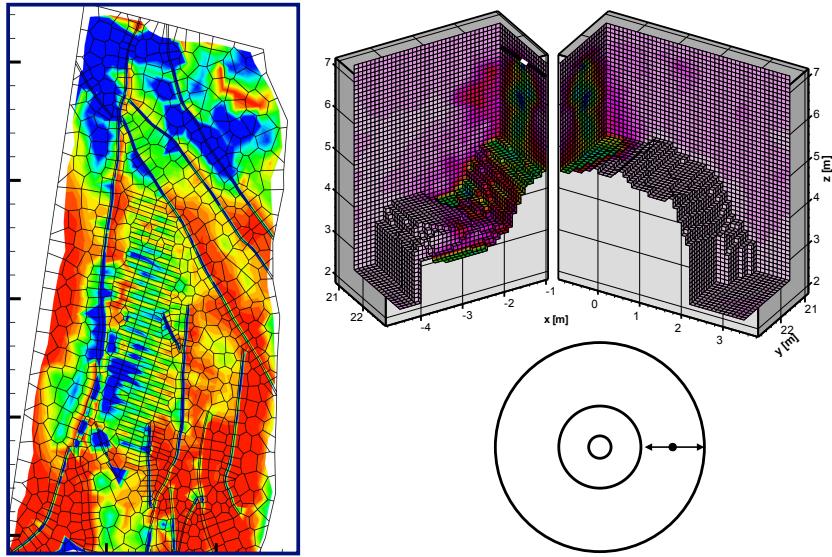
Voronoi Grid

- Structured / unstructured grids
- Locally one-dimensional
- No reference to global coordinate system
- Orthogonality requirement!



4

Examples of Voronoi Grids



Element / Gridblock

- TOUGH2 block ELEME
- Element name (format: A3I2, e.g., ELE99)
- Material type / material number (see block ROCKS)
- Volume [m³]
- Optional:
 - Interface area to heat-conducting, confining layer
 - permeability modifier
 - X-, Y- and Z-coordinates

```
ELEMEE-----1-----2-----3-----4-----5-----6-----7-----8
A11 1           SOIL   0.100E-09 0.100E+01          0.500E+00 0.500E+00 -0.500E-10
A21 1           FRACT  0.500E-01          0.500E+00 0.500E+00 -0.250E-01
A31 1           7 0.500E-01          0.500E+00 0.500E+00 -0.750E-01
.....
Name       Material    Volume    (AHTX)     (PMX)     (X)     (Y)     (Z)
```

6

Connections

- TOUGH2 block CONNE
- A connection connects *two* elements
- Elements can have multiple connections
- **Names of two elements (A3I2 A3I2)**
- Anisotropy index (permeability index 1, 2, or 3, see ROCKS)
- Nodal distances [m] from each element to interface
- Interface area [m^2]
- Cosine of angle between gravity vector and connection line

```

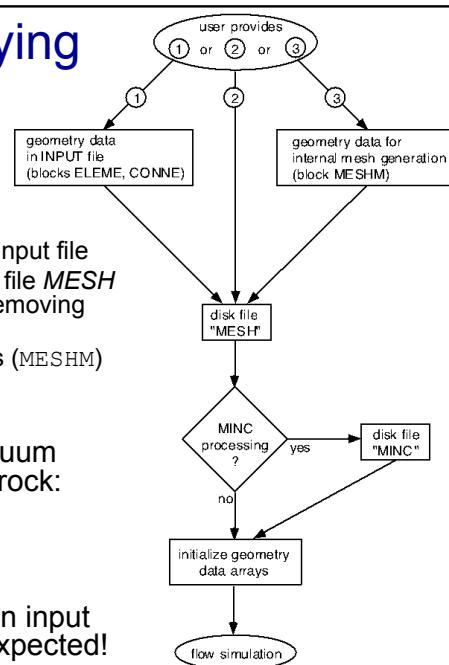
CONNE---1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
A11 1A21 1          1 0.500E-10 0.250E-01 0.100E+01 0.000E+00
A21 1A31 1          2 0.250E-01 0.250E-01 0.100E+01
A31 1A41 1          3 0.250E-01 0.250E-01 0.100E+01 -.100E+01
...
Element 1 and 2      ISOT     D1      D2      AREAX      BETAX

```

7

Options for Supplying Geometry Data

- Three options:
 - Blocks ELEME and CONNE in input file
 - Blocks ELEME and CONNE on file MESH (remove ‘+++’ if adding/removing elements or connections!)
 - Use internal mesh generators (MESHM)
 - XYZ
 - RZ2D
- MINC processing for continuum representation of fractured rock:
 - double-porosity
 - dual-permeability
 - multiple interacting continua
- If no ELEME block is found in input file, external file MESH is expected!



8

TOUGH

Training Courses



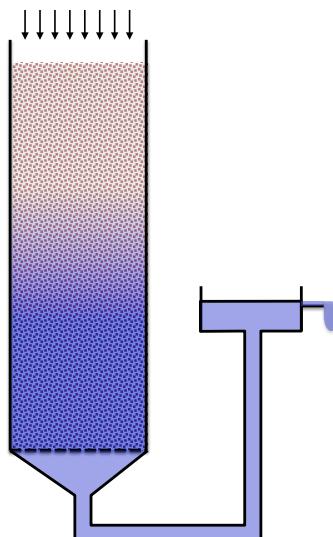
Exercise 1b

- ✓ Rock Properties
- Mesh Generation
- Initial and Boundary Conditions
- Computational Parameters

9

Model Domain

- Drainage experiment in 1-m long laboratory column filled with homogeneous sand
- Generate mesh using MESHMAKER
- Consider boundary conditions:
 - initially fully saturated, hydrostatic
 - constant pressure at bottom during subsequent drainage experiment
 - open to atmosphere at top
- Assign materials to elements



10

MESHSMaker

- Approach:
 - Use TOUGH2's built-in mesh generator MESHSMaker
 - Learn about blocks ELEME and CONNE
 - Modify mesh
 - Input file: *P1b.txt*
 - Output files: *P1b.out*, *MESH*

11

MESHSMaker XYZ

```
Plb: Generating a 1D mesh for simulating column experiment
MESHM---1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
XYZ
                                Specify orientation
NX      1      ?.?      Select dX and dY to yield cross section of column
NY      1      ?.?
NZ      1      1.0E-06     Add (dummy) top boundary element
NZ      20      ?.??     Create uniform grid for 1 m long column
NZ      1      1.0E-06     Add (dummy) bottom boundary element
                                Needs one empty line to terminate XYZ block
                                Needs another empty line to terminate MESHSMAKER
ENDFI---1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
```

- Consult Appendix F of TOUGH2 Manual
- Open file *P1b.txt* using a text editor
- Replace **???** in input file
- Answer following questions *before* running TOUGH2:

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Questions MESHMAKER

- Q1: Line 1: Is it necessary to provide a title line? _____
- Q2: Why do you have to specify NX, NY, and NZ for a 1D problem? _____

- Q3: What value did you select for dX and dY, and why?

- Q4: Why do you need to specify dummy boundary elements?

13

Questions MESHMAKER

- Q5: Why is a small dZ for the boundary elements recommended? _____

- Q6: What vertical grid resolution did you pick?

- Q7: What is the difference between the keywords ENDFI and ENDCY? _____

14

Run *P1b.txt*

- Open a DOS command prompt window:

START → Programs → Accessories → Command Prompt
or

START → Run → enter: cmd

- Change directory to Short Course directory:

cd ...\\Problems\\Problem_Tutorial

- Run TOUGH2 by typing:

xt2_eos9 < P1b.txt > P1b.out

- Open the following output files:

MESH

P1b.out

15

Output File *MESH*

ELEM		
A11 1	10.1000E-090.1000E+01	0.5000E+000.5000E+00-.5000E-10
A21 1	10.5000E-010.0000E+00	0.5000E+000.5000E+00-.2500E-01
A31 1	10.5000E-010.0000E+00	0.5000E+000.5000E+00-.7500E-01
A41 1	10.5000E-010.0000E+00	0.5000E+000.5000E+00-.1250E+00
.....
AJ1 1	10.5000E-010.0000E+00	0.5000E+000.5000E+00-.8750E+00
AK1 1	10.5000E-010.0000E+00	0.5000E+000.5000E+00-.9250E+00
AL1 1	10.5000E-010.0000E+00	0.5000E+000.5000E+00-.9750E+00
AM1 1	10.1000E-090.1000E+01	0.5000E+000.5000E+00-.1000E+01
CONNE		
A11 1A21 1	30.5000E-100.2500E-010.1000E+010.1000E+01	
A21 1A31 1	30.2500E-010.2500E-010.1000E+010.1000E+01	
A31 1A41 1	30.2500E-010.2500E-010.1000E+010.1000E+01	
A41 1A51 1	30.2500E-010.2500E-010.1000E+010.1000E+01	
.....
A11 1AJ1 1	30.2500E-010.2500E-010.1000E+010.1000E+01	
AJ1 1AK1 1	30.2500E-010.2500E-010.1000E+010.1000E+01	
AK1 1AL1 1	30.2500E-010.2500E-010.1000E+010.1000E+01	
AL1 1AM1 1	30.2500E-010.5000E-100.1000E+010.1000E+01	

16

Questions MESHMAKER

- Q8: Confirm that the calculated element volume is consistent with the expected value. _____

- Q9: What is the nodal distance from one element to the interface, and what is the interface area? _____

- Q10: How can you tell (from the CONNE block!) that element A21 1 is *above* element A31 1? _____

17

Assign Materials

- Open file *MESH* generated by Exercise 1b
- Assign materials to each element (either by name or number) according to the ROCKS block of Exercise 1a
- Save the modified *MESH* file for Exercise 1c

18



Training Courses



Initial and Boundary Conditions

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Outline Initial and Boundary Conditions

- General Concept
- Block **PARAM. 4**
- Block **INDOM**
- Block **INCON**
- Block **GENER**
- *Exercise 1c*

2

1

General Concept

- Primary variables *completely* define the **system state**
- Choice of primary variables defines the **phase state** (single-phase vs. two-phase conditions)
- **Initial conditions** are the set of primary variables at the beginning of a simulation
- **Dirichlet boundary conditions** are given as *initial conditions* for inactive elements (or elements with a very large volume)
- The system state at the end of a simulation (stored on file *SAVE*) can be used as the initial conditions (file *INCON*) for a subsequent simulation

3

Primary Variables – Secondary Parameters

- The **primary variables** are the time-dependent *unknowns* of the simulation, i.e., they are the *solution variables*
- Within an element, *local thermodynamic equilibrium* is assumed; consequently, the number of primary variables is equal to NK mass balance equations and one energy balance equation
- The number of primary variables depends on EOS module (e.g., EOS9: 1; EOS1-5: 3; EOS7R: 6; T2VOC: 4)
- **Secondary parameters** are fluid and state-related *properties* calculated as a function of the system state, i.e., sec. par. = $f(\text{prim. variables})$

4

Variable Switching

- Each element may be in a different phase state, i.e., may have a different set of primary variables
- Phase state may change during simulation (phase appearance/disappearance) → **variable switching**
- Primary variables are identified by their *position and value* (sometimes a constant 10 is added)
- *First* primary variable is (gas) **pressure**;
Exception: EOS9 unsaturated conditions
- *Last* primary variable is always **temperature** (even if isothermal conditions are chosen)
Exception: EOS1, EOS2, EOS4, EOS9

5

Single-Phase vs. Two-Phase Conditions for EOS3 (1 of 3)

- (Second) primary variable for *single-phase* conditions is air-mass fraction in phase β , X_{β}^{air}
- (Second) primary variable for *two-phase* conditions is saturation $S_g + 10$
- 10 is added to S_g to distinguish between single- and two-phase conditions based on the numerical value alone:
$$0 \leq X_{\beta}^a \leq 1 \quad \text{and} \quad 0 + 10 < S_g + 10 < 1 + 10$$
- What is β in X_{β}^{air} , *l* (liquid) or *g* (gas)?
- How can we distinguish between single-phase *liquid* and single-phase *gas*?

6

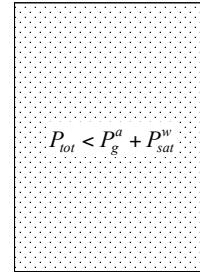
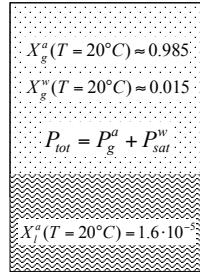
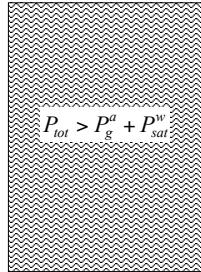
Single-Phase vs. Two-Phase Conditions (2 of 3)

- **Single-phase liquid:** $0 \leq X_{\beta}^a = X_l^{\text{air}} < X_{l,\text{eq}}^{\text{air}}$
 - Value of X_{β}^{air} typically close to zero
 - Represents amount of air dissolved in liquid phase
 - Solubility limit $X_{l,\text{eq}}^{\text{air}}$ given by **Henry's law**
 - Typical value (P = 1 bar, T = 20°C): $X_{l,\text{eq}}^{\text{air}} \approx 1.6 \times 10^{-5}$
- **Single-phase gas:** $X_{g,\text{eq}}^{\text{air}} < X_{\beta}^a = X_g^{\text{air}} \leq 1$
 - Value of X_{β}^{air} typically close to one
 - Represents amount of air present in gas phase
 - $X_{g,\text{eq}}^{\text{air}} = 1 - X_{g,\text{eq}}^w$ given by **vapor pressure curve**
 - Typical value (P = 1 bar, T = 20°C): $X_{g,\text{eq}}^{\text{air}} \approx 0.985$
- **Two-phase:** $X_l^{\text{air}} = X_{l,\text{eq}}^{\text{air}}$ and $X_g^{\text{air}} = X_{g,\text{eq}}^{\text{air}}$
 - X_{β}^{air} at equilibrium values determined by P and T
 - X_{β}^{air} no longer a prim. variable → initialize as $S_g + 10$

7

Single-Phase vs. Two-Phase Conditions (3 of 3)

$$\text{Mass fraction: } X_{\beta}^{\kappa} = \frac{m_{\beta}^{\kappa}}{m_{\beta}} = \frac{m_{\beta}^{\kappa}}{\sum_{\kappa=1}^{NK} m_{\beta}^{\kappa}} = \frac{x_{\beta}^{\kappa} M^{\kappa}}{\sum_{\kappa=1}^{NK} x_{\beta}^{\kappa} M^{\kappa}} \quad \sum_{\kappa=1}^{NK} X_{\beta}^{\kappa} = 1 \quad M^{\kappa} = m^{\kappa} / n$$



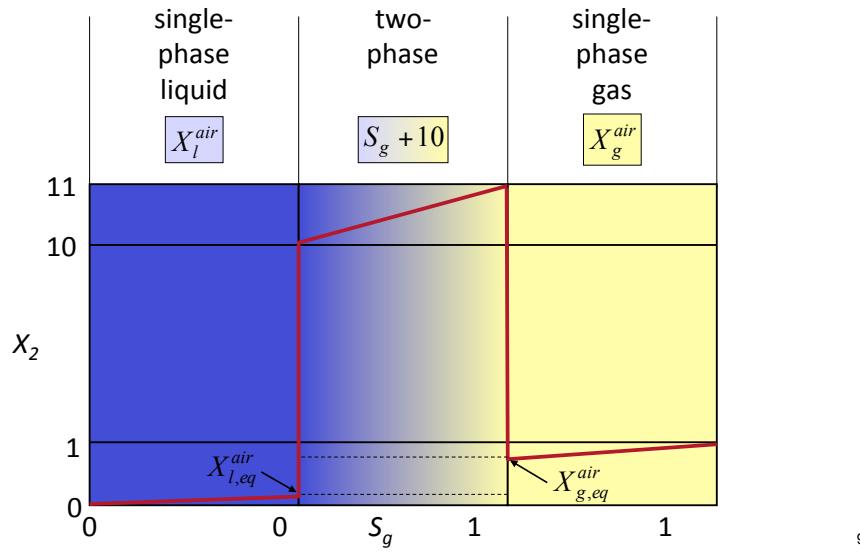
Single-phase liquid
 P_{tot}, X_l^a, T

Two-phase gas-liquid
 $P_g, 10+S_g, T$

Single-phase gas
 P_g, X_g^a, T

8

Variable Switching



Specifying Initial Conditions

- Provide *default* initial conditions in block `PARAM.4`:
 - Apply to all elements
- Provide *domain-specific* initial conditions in block `INDOM`
 - Provide domain name from `ROCKS` and primary variables
 - Overwrites default values given through `PARAM.4`
- Provide *element-specific* initial conditions in block `INCON`
 - Provide element name and primary variables
 - Overwrites default and domain specific primary variables
- Provide keyword `START` if `INCON` does *not* provide initial conditions for *all* elements in *same order* as block `ELEME`
- File `SAVE` contains `INCON` block to be used for follow-up run
- Block `INCON` may be provided on external file `INCON`

10

Example: EOS3

Primary Variables
 X(1) X(2) X(3)

Two-Phase Conditions: P_g S_g+10 T

Single-Phase Conditions: P X_{β}^{air} T

```

PARAM---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
 8 2   10      1100000100000000400001000
          1.000E+10 1.000E-01           9.81
 1.000E-05
          10130.0           1.E-5        20.0

INDOM---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
BOUND
          20000.0           0.983       35.0

INCON---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
ELM 1      0.35
          10130.0           10.65       20.0
ERR 0      0.99
          10130.0           0.70        20.0
  
```

11

How to find out mass fractions $f(P,T)$ and thermophysical properties?

- Create TOUGH2 model consisting of a single element
- Initialize element with **two-phase conditions** at desired pressure and temperature
 - because of the local thermodynamic equilibrium assumption, selecting two-phase conditions implies that the gas phase is at **100% relative humidity** (i.e., $P_g^w = P_{\text{sat}} \rightarrow X_g^w = X_{g,\text{eq}}^w$), and the NCG dissolved in the liquid phase is at its **solubility limit** (i.e., $X_l^{\text{NCG}} = X_{l,\text{eq}}^{\text{NCG}}$)
- Set MOP (5) = 9 to get a printout of all the secondary parameters
- Perform a “simulation” with a tiny time step; check output
- *Such a model is provided, with predefined primary variables for all EOS modules (see next slide)*

12

13

```

PRIMARY VARIABLES
AT ELEMENT *1PH01* --- 0.300000E+08 0.000000E+00 0.500000E+02
AT ELEMENT *2PH02* --- 0.100000E+06 0.105000E+02 0.200000E+02

SECONDARY PARAMETERS
Secondary parameter in order shown in Figure 3 of manual:
ELEMENT 1PH01
0.000000E+00 0.000000E+00 0.100000E+01 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.100000E+02
0.547260E-03 0.100072E+04 0.234951E+06 -0.000000E+00 0.100000E+01 0.000000E+00 0.500000E+02 0.000000E+00

0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.103377E-12 0.408132E-06 0.852618E-03 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00

0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 -0.100000E+01 0.100000E+01 0.000000E+00 0.000000E+00

0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
-0.913807E-05 -0.454514E+00 0.411725E+04 0.000000E+00 0.000000E+00 0.000000E+00 0.100000E+01 0.000000E+00

ELEMENT 2PH02
0.500000E+00 0.433913E+00 0.181347E-04 0.117767E+01 0.134637E+06 0.000000E+00 0.146811E-01 0.985319E+00 0.500000E+00 0.896327E-02
0.100174E-02 0.998323E+03 0.839536E+05 -0.000000E+00 0.999984E+00 0.156989E-04 0.200000E+02 0.253818E+07

.....
```

gas

liquid

t2: Two-element problem to check thermophysical properties and primary variables

THE TIME IS 0.11574E-14

OUTPUT DATA AFTER (1, 1) -2-TIME STEPS

ELEM.	INDEX	P (PA)	T (DEG-C)	SG	SL	XAI RG	XAI RL	PSAT (PA)	PCAP (PA)	DG (KG/M^3*	LOG (PERM)
1PH01	1	3000000.00	50.00000	0.00000	1.00000	0.00000E+00	0.00000E+00	0.12335E+05	-0.00000E+00	0.00000	-14.00000
2PH02	2	100000.00	20.00000	0.50000	0.50000	0.98532E+00	0.156989E-04	0.23366E+04	-0.00000E+00	1.17767	-14.00000

14

14

Dirichlet Boundary Conditions

- Constant pressure/saturation/temperature boundary conditions are specified as *initial conditions*
- To keep them constant, do one of the following:
 - Set the corresponding boundary element *volume* to a *very large* value (typically 1.0E50). The very large volume ensures that the system state in this element remains constant despite inflow/outflow of fluids and energy; or
 - Make boundary elements *inactive* by moving them to the end of block ELEME, *after* an element of zero or *negative volume*
- Specify **constant temperature boundary conditions** (but variable pressure/saturation) by setting rock *grain density* to a very large value (typically 1.0E50)

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Neumann Boundary Conditions

- Specified flow (Neumann) boundary conditions are specified through block GENER
- Neumann boundary conditions can be *constant* or *time-dependent* (tabular input)
- *Injection is positive, production is negative*
- For **injection**, specify mass flow rate of *component κ* (*not phase β*) and enthalpy
- For **production**, specify *total mass* of produced fluid mixture
- *Phase composition* for production is determined by phase composition and mobility of producing element (see also MOP (9))

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Example GENER

- Injection: Specify component mass
- Production: Specify total mass
- Time dependent: Provide LTAB table entries
- MOP (9): Composition of produced fluid
- MOP (12): Interpolation for time dependent sink/source data
- See Manual for additional options (e.g., wells on deliverability, heat injection, etc.)

```
GENER----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6
ELM 1INJ 1                               WATE      1.0
ELM 1INJ 2                               COM2      1.6E-5
ELM 2PRO 1                               MASS      -0.2
ELM10PRO10          4                  MASS
                                         0.0      3600.0     3610.0     86400.0    ← time
                                         -0.2       -0.2       -0.5       -1.3    ← rate
```

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Atmospheric Boundary (1 of 5)

- No atmospheric boundary element needed for Richards equation (EOS9)
- Specify Dirichlet boundary condition at land surface (i.e., inactive element or element with large volume; special rock type, e.g., ATMOS)
- A single atmospheric element can be connected to all elements at the ground surface (use, e.g., [AddBound.exe](#))
- Use small nodal distance (e.g., boundary layer thickness) from atmospheric element to interface with first row of soil elements

18

Atmospheric Boundary (2 of 5)

- Initial condition in atmospheric element:
 - Atmospheric pressure and temperature
 - For **100% relative humidity**, use **two-phase** point with liquid saturation smaller than residual liquid saturation (so relative permeability is zero, preventing liquid flow into soil)
 - For **less than 100% relative humidity**, use **single-phase gas** point with appropriate air mass fraction X_g^a ($X_g^a=1.0$ for dry air; minimum value $X_{g,min}^a=1-X_{g,eq}^w$ depends on vapor pressure (which is a function of temperature); intermediate values $X_{g,min}^a(T) < X_g^a \leq 1.0$ determine relative humidity)

19

Atmospheric Boundary (3 of 5)

- Material Properties for Atmosphere
 - Select relative permeability and capillary pressure functions so that (for the saturation given in the atmospheric boundary element):
 - Liquid relative permeability is **zero** at specified saturation
 - Gas relative permeability is **one** at specified saturation
 - Capillary pressure is **zero** at specified saturation
 - Ensure **upstream weighting** of mobilities (see MOP (11))
- Infiltration
 - Specify infiltration rates in row of elements **below** the atmospheric boundary element using the **GENER** block
- Evaporation
 - Simulate as **binary diffusion** process (atmosphere at <100% r.h.)
 - Specify ET rate in row of elements **below** the atmospheric boundary element using the **GENER** block
 - Assign capillary pressure according to **Kelvin's equation** in atmospheric element (see Ghezzehei et al., *Vadose Zone J.*, 3: 806–818, 2004)

20

10

Atmospheric Boundary (4 of 5)

Dirichlet atmospheric b.c.:

Two-phase for 100% r. h.
 $S_{l,initial} = 0.01 < S_{lr}$
 Single-phase gas for < 100% r.h.
 $X_{g,min}(T) < X_g^a \leq 1.0$

Neumann b.c.:

GENER, with rates
 positive for infiltration and
 negative for ET

$P_{cap} = 0$
 $k_{rl} = 0$
 $k_{rg} = 1$

} for $S_l = S_{l,initial}$

$V = 1E50$ or inactive element

$d1 = \text{small}$

\circ \circ

A11 1 A2150

A31 1• A31 2• A31 3◦ A3150

A41 1• A41 2• A41 3◦ A4150

• • ◦

• • ◦

21

Atmospheric Boundary (5 of 5)

```

ROCKS---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
ATMOS   2      2650.    .9999          1.000E-12    2.51    100000.
                                1.0
                                1     0.1     0.0     1.0     0.1
                                1     0.0     0.0     1.0
SOIL    0      2650.    .3000 1.000E-12 1.000E-12 1.000E-12    2.51     920.

ELEM
A11 1    ATMOS 0.1000E+510.1000E+01          0.0
A21 1    SOIL  0.5000E-010.0000E+00          0.5000E+000.5000E+00-.2500E-01
A31 1    SOIL  0.5000E-010.0000E+00          0.5000E+000.5000E+00-.7500E-01
.....
A2150   SOIL  0.5000E-010.0000E+00          0.1000E+010.5000E+00-.2500E-01
A3150   SOIL  0.5000E-010.0000E+00          0.1500E+010.5000E+00-.7500E-01
.....

```

```

CONN
A11 1A21 1    30.5000E-020.2500E-010.1000E+010.1000E+01
A11 1A21 2    30.5000E-020.2500E-010.1000E+010.1000E+01
.....
A11 1A2150   30.5000E-020.2500E-010.1000E+010.1000E+01
.....
A2250A3150   30.2500E-010.2500E-010.1000E+010.1000E+01
.....

```

```

INCON---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
A11 1           1.013E5          10.99          20.0

```

```

GENER---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
A21 1INF 1     49       1       1          WATE     1.0E-4

```

22



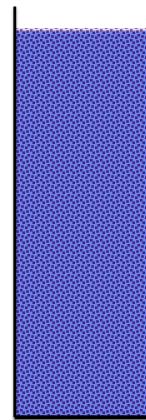
Exercise 1c

- ✓ Rock Properties
- ✓ Mesh Generation
- Initial and Boundary Conditions
- Computational Parameters

23

Exercise 1c: Define Initial and Boundary Conditions; Calculate Hydrostatic Profile

- Define initial and boundary conditions:
 - Column is initially fully liquid saturated
 - Column is open to atmosphere (1 bar) at top
 - Column is closed at bottom
 - No infiltration ($q=0$)
- Create hydrostatic profile



24

Questions Primary Variables (general)

Q1: To fully define the system state, how many variables are needed
(a) in general, and (b) specific for Exercise 1?

(a) _____

(b) _____

Q2: Identify primary variables and corresponding phase state for EOS9.

Q3: The first primary variable in an EOS9 simulation is given as 0.75.
What is (a) the liquid saturation, (b) the gas pressure, and (c) the
liquid pressure in that element?

(a) _____

(b) _____

(c) _____

25

Questions Hydrostatic Profile Run

Q4: What pressure do you expect at the bottom of
the column?

Q5: Calculate (a) the total volume and (b) the total
mass of liquid you expect in the column

(a) _____

(b) _____

26

Initial and Boundary Conditions

- Edit file *P1c.txt* (see next slide)
- Specify appropriate initial and boundary conditions for the simulation of a hydrostatic pressure profile under fully liquid saturated conditions
- To implement initial and boundary conditions, modify (as necessary) blocks **PARAM.4**, **INDOM**, **INCON**, and **ELEME**

27

P1c.txt

```
P1c: Create hydrostatic pressure profile
Copy block ROCKS from Exercise P1a here:
???

Copy block RPCAP from Exercise P1a here:
???

Provide default initial condition in block PARAM.4
PARAM----1--MOP(123456789012345678901234)---*---5---*---6---*---7---*---8
 8 2 100      1100000900000000400001000
          86400.0 1.000E-01           10.0
 1.000E-07
???


Copy blocks ELEME and CONNE (i.e., file MESH) from Exercise P1b here.
Assign materials (either by name or number) to each element.
Consider changing volumes of boundary elements.

???


START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
Consider making changes to blocks INDOM and/or INCON
INDOM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
???


INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
???


ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

28

Run Exercise 1c

- Run file *P1c.txt*
- Open output file *P1c.out* and answer the questions on the following slides

(Note: The sequence of the questions is such that the answers can be found by reading the output file from top to bottom. The main purpose of this exercise is to get familiar with a typical TOUGH2 output file.)

29

Questions TOUGH2 Output File *P1c.out*

Q6: What is the maximum number of elements and connections you could handle with this installation of TOUGH2?

Q7: How many significant digits are there?

Q8: How many active elements and connections are there in your model?

30

Questions TOUGH2 Output File *P1c.out*

Q9: What is the value of acceleration of gravity?

Q10: What initial condition was assigned to element
A11 1? _____

Q11: What water property values are used?

31

Questions TOUGH2 Output File *P1c.out*

Q12: What is the initial total volume and mass of
liquid in the system?

Q13: What is the size of the first time step?

Q14: What is the flow rate of water into the column
after the first time step?

32

Questions TOUGH2 Output File *P1c.out*

Q15: After how many time step was steady state reached? _____

Q16: Describe the pressure profile

Q17: What is the liquid saturation in element A11 1?

Q18: Check file *SAVE*. What does it contain?

33



Nonlinear and Linear Solvers

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Outline

- Newton-Raphson iterations
- Linear equation solvers
- Weighting schemes

2

1

Integral Finite Difference Method

- In the **Integral Finite Difference** (IFD) method, space discretization is made directly from the integral equations:

$$\frac{d}{dt} \int_{V_n} M^\kappa dV_n = \oint_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^\kappa dV_n$$

(i.e., no PDE is derived and then integrated)

3

Mass Balance Equation in Discretized Form

4

2

Balance Equation for Multiphase-Multicomponent System

- Balance Equation for Component κ [kg s⁻¹]:

$$\frac{d}{dt} \int_{V_n} M^\kappa dV_n = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^\kappa dV_n$$

- Specific Mass [kg m⁻³]:

$$M^\kappa = \phi \sum_\beta S_\beta \cdot \rho_\beta \cdot X_\beta^\kappa$$

- Specific Advective Mass Flux [kg m⁻² s⁻¹]:

$$\mathbf{F}^\kappa = \sum_\beta X_\beta^\kappa \cdot \mathbf{F}_\beta$$

$$\mathbf{F}_\beta = \rho_\beta \mathbf{u}_\beta = -k \frac{k_{r\beta} \rho_\beta}{\mu_\beta} (\nabla P_\beta - \rho_\beta \mathbf{g})$$

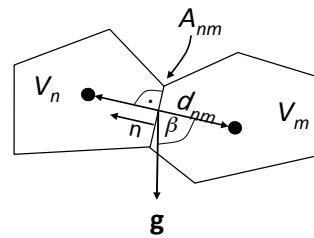
- See Appendix D for multiphase diffusion

5

Spatial Discretization

- Accumulation Term [kg]:

$$\int_{V_n} M^\kappa dV_n = V_n \cdot M^\kappa = V_n \cdot \phi \left(\sum_\beta S_\beta \cdot \rho_\beta \cdot X_\beta^\kappa \right)$$



- Advective Flux Term [kg s⁻¹]:

$$\oint_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma = \sum_m A_{nm} \cdot F_{nm}^\kappa = \sum_m A_{nm} \cdot \left[\sum_\beta X_\beta^\kappa \cdot F_\beta \right]_{nm} = \\ \sum_m A_{nm} \cdot \left[\sum_\beta X_\beta^\kappa \cdot k_{nm} \left(\frac{k_{r\beta} \cdot \rho_\beta}{\mu_\beta} \right)_{nm} \cdot \left(\frac{P_{\beta m} - P_{\beta n}}{d_{nm}} + \rho_{\beta nm} \cdot g \cdot \cos \beta_{nm} \right) \right]$$

- Sink/Source Term [kg s⁻¹]:

$$\int_{V_n} q^\kappa dV = q_n^\kappa \cdot V_n = Q_n^\kappa$$

6

Temporal Discretization

- First-order differential equation in time [kg m⁻³ s⁻¹]:

$$\frac{dM_n^{\kappa}}{dt} = \frac{1}{V_n} \left(\sum_m A_{nm} \cdot F_{nm}^{\kappa} + V_n \cdot q_n^{\kappa} \right)$$

- Implicit time discretization (k is time index):

$$\frac{(M_n^{\kappa,k+1} - M_n^{\kappa,k})}{\Delta t} = \frac{1}{V_n} \cdot \left(\sum_m A_{nm} \cdot F_{nm}^{\kappa,k+1} + V_n \cdot q_n^{\kappa,k+1} \right)$$

- Nonlinear algebraic residual equations [kg m⁻³]:

$$R_n^{\kappa,k+1} = (M_n^{\kappa,k+1} - M_n^{\kappa,k}) - \frac{\Delta t}{V_n} \left(\sum_m A_{nm} F_{nm}^{\kappa,k+1} + V_n \cdot q_n^{\kappa,k+1} \right) \equiv 0$$

7

Nonlinearity: Newton-Raphson Iteration

- Taylor series expansion of residual equation for x_i (p is NR-iteration index):

$$R_n^{\kappa,k+1}(x_{i,p+1}) = R_n^{\kappa,k+1}(x_{i,p}) + \sum_i \left. \frac{\partial R_n^{\kappa,k+1}}{\partial x_i} \right|_p (x_{i,p+1} - x_{i,p}) + \dots = 0$$

- Equation for increment:

$$-\sum_i \left. \frac{\partial R_n^{\kappa,k+1}}{\partial x_i} \right|_p (x_{i,p+1} - x_{i,p}) = R_n^{\kappa,k+1}(x_{i,p})$$

- Set of linear equations:

$$[\mathbf{J}_p] \cdot [\Delta \mathbf{x}_p] = [\mathbf{R}_p]$$

- Jacobian matrix:

$$J_{ij} = -\frac{\partial R_i^{k+1}}{\partial x_j}$$

- Convergence criterion:

$$\left| \frac{R_{n,p+1}^{\kappa,k+1}}{M_{n,p+1}^{\kappa,k+1}} \right| \leq \varepsilon$$

8

Linear Equation Solvers

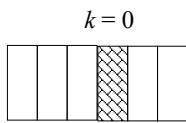
- Solve $[\mathbf{J}] \cdot [\Delta \mathbf{x}] = [\mathbf{R}]$ for each Newton-Raphson iteration
- Direct solver (LUBAND): robust, but inefficient
- Iterative solvers (see MOP (21) and SOLVR)
 - DSLUBC, a bi-conjugate gradient solver
 - DSLUCS, a Lanczos-type bi-conjugate gradient solver
 - DSLUGM, a generalized minimum residual solver
 - DLUSTB, a stabilized bi-conjugate gradient solver
- Preconditioning (Z- and O-preconditioning; see SOLVR)
- Parallelization (domain partitioning; AZTEC or PETSc parallel solvers)

9

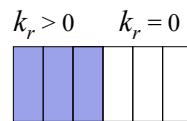
Evaluation of Interface Terms

$$F_{nm}^\kappa = \left[\sum_\beta X_\beta^\kappa \cdot k_{nm} \left(\frac{k_{r\beta} \cdot \rho_\beta}{\mu_\beta} \right)_{nm} \cdot \left(\frac{P_{\beta m} - P_{\beta n}}{d_{nm}} + \rho_{\beta nm} \cdot g \cdot \cos \beta_{nm} \right) \right]$$

- $k, k_{r\beta}, \rho_\beta, \mu_\beta$ need to be evaluated at interface nm
- **How to average?**
 - Harmonic mean for k
 - Upstream weighting for mobility k_r/μ :
 - Upstream for ρ in mobility term; arithmetic mean in gravity term



$$k_{i-1/2} = \frac{2k_{i-1}k_i}{k_{i-1} + k_i}$$



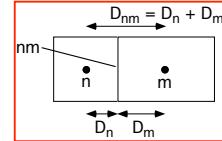
$$k_{r,i-1/2} = k_{r,i-1}$$

10

Harmonic Weighting

Simplify notation by abbreviating $K_{nm} = k_{nm} \left[\frac{\rho}{\mu} \right]_{nm}$

Then have $F_{nm} = K_{nm} \left[\frac{P_m - P_n}{D_{nm}} \right]$



Introduce the (unknown) fluid pressure P_{nm} at the interface and write

$$F_{nm} = K_m \left[\frac{P_m - P_{nm}}{D_m} \right] = K_n \left[\frac{P_{nm} - P_n}{D_n} \right]$$

Setting this equal to the above flux expression gives two equations for the two unknowns P_{nm} and K_{nm} :

$$\frac{D_m}{K_m(P_m - P_{nm})} = \frac{D_{nm}}{K_{nm}(P_m - P_n)}$$

$$\frac{D_n}{K_n(P_{nm} - P_n)} = \frac{D_{nm}}{K_{nm}(P_m - P_n)}$$

Multiply the first equation with $(P_m - P_{nm})$, the second with $(P_{nm} - P_n)$ and add:

$$\frac{D_m}{K_m} + \frac{D_n}{K_n} = \frac{D_{nm}(P_m - P_{nm} + P_{nm} - P_n)}{K_{nm}(P_m - P_n)} = \frac{D_{nm}}{K_{nm}}$$

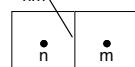
“harmonic weighting”

11

Upstream Weighting

How do we proceed in more complicated circumstances? For example, consider solute transport (C = concentration).

$$\mathbf{F}^\kappa = -k \frac{\rho}{\mu} C \nabla P \quad F_{nm}^\kappa = k_{nm} \left[\frac{\rho}{\mu} \right]_{nm} C_{nm} \left[\frac{P_m - P_n}{D_{nm}} \right]$$



One might think of interpolating, $C_{nm} = \frac{1}{2}(C_n + C_m)$

However...

Let us suppose flow is from m to n , and $C_m < C_n$. Then $C_{mn} > C_m$, and by flowing from m to n we would remove fluid from m that has a higher concentration than is present in m . Concentrations in m could even become negative, for example when $C_m = 0$. Similar considerations apply for heat flow: we could be transferring heat from the colder region to the hotter one, while cooling the colder region, in violation of the Second Law of Thermodynamics.

To avoid this kind of unphysical behavior, employ “total variation diminishing” (TVD) interpolation schemes. The simplest such scheme is “**upstream weighting**”:

$$C_{nm} = \begin{cases} C_m & \text{if flow is from } m \text{ to } n \\ C_n & \text{if flow is from } n \text{ to } m \end{cases}$$

12

Interface Weighting (MOP (11))

transient two-phase flow	
uniform medium	composite medium
k (constant) k_r (upstream)	k k_r } upstream
steady two-phase flow	
k k_r harmonic	
single-phase flow	
k harmonic k_r (none)	

13

Final Comments on IFD

- Advantages
 - Physical, intuitive
 - Irregular grids
 - 0D, 1D, 2D, 3D, radial, spherical, ... (IFD is **locally 1D!**)
 - **fractured** systems implemented through geometry only
 - Easy implementation of boundary conditions
 - No reference to global coordinate system
 - Locally and globally **mass conservative**
- Difficulties
 - Tensors
 - Higher-order schemes
 - Normality requirement (Voronoi)

14



Computational Parameters

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Outline Computational Parameters

- General concept
- Time stepping
- Convergence criteria
- Weighting schemes
- Controlling output
- Solver options
- Miscellaneous
- *Exercise 1d*

2

1

General Concept

- A TOUGH2 simulation is controlled by program options, time stepping and convergence parameters
- Computational parameters are provided through a number of input blocks:
 - MULTI
 - PARAM
 - SOLVR
 - ENDFI, ENDGY
- Time stepping parameters are provided through blocks:
 - PARAM
 - (TIMES)
- Printout options are provided through blocks:
 - PARAM
 - TIMES
 - FOFT, COFT, GOFT
 - NOVER

3

Block MULTI

- Specifies number of fluid components; selects isothermal vs. nonisothermal and diffusion options
- Available options are EOS-specific (check TOUGH manual, Section 6, or output file)
- Selects isothermal vs. nonisothermal simulations:
 - If $NEQ = NK$: isothermal
 - If $NEQ = NK + 1$: nonisothermal
- Used to include diffusion:
 - If $NB = 6$: no diffusion
 - If $NB = 8$: include diffusion
- Used to select number of primary variables (NKIN) in INCON block (only certain EOS modules)

```
MULTI----1-----*----2-----*----3  
      2   3   2   6  
  
      NK    NEQ    NPH    NB  (NKIN)
```

4

Simulation Time, Block PARAM

Variable	Description	Default
MCYC	Maximum number of time steps	-
TSTART	Starting time of simulation	0
TIMAX	Ending time of simulation	∞

```

MOP (i,i=1,24)
PARAM---1----*-123456789012345678901234----*---5----*---6----*---7
8 2 100      5100000100000000400001000
     0.0    86400.0      1.0     3600.0      9.81
 1.000E-05      1.0      1.0      1.0      1.0E-8
           1.0E+05      10.35      20.0

```

5

Time-Step Control

Variable	Description	Default
DELTEN	Initial time step size	-
DELMX	Maximum time step size	∞
MOP (16)	Double time step if $n_{NR} \leq MOP (16)$	-
NOITE	Reduce time step by REDLT if $n_{NR} > NOITE$	8
REDLT	Time-step reduction factor	4.0

Block TIMES :

Simulation lands on printout times, affecting time-step size

```

MOP (i,i=1,24)
PARAM---1----*-123456789012345678901234----*---5----*---6----*---7
8 2 100      5100000100000000400001000
     0.0    86400.0      1.0     3600.0      9.81      4.0
 1.000E-05      1.0      1.0      1.0      1.0E-8
           1.0E+05      10.35      20.0

```

6

Newton-Raphson Iterations and Linear Equation Solver

Variable	Description	Default
MOP (1)	Create printout for non-convergent iterations Recommendation: set MOP (1)>0	no
MOP (21)	Select linear equation solver	3
RE1	Relative error convergence criterion	1.0E-5
RE2	Absolute error convergence criterion	1.0
WNR	Weighting factor for N-R increment	1.0

Check block SOLVR for preconditioners and other options
Check file LINEQ for linear equation solver information

```

MOP (i,i=1,24)
PARAM---1----*-123456789012345678901234----*---5----*---6----*---7
 8 2 100      5100000100000000400003000
    0.0   86400.0      1.0   3600.0      9.81      4.0
 1.000E-05     1.0          1.0      1.0   1.0E-8
           1.0E+05      10.35      20.0

```

7

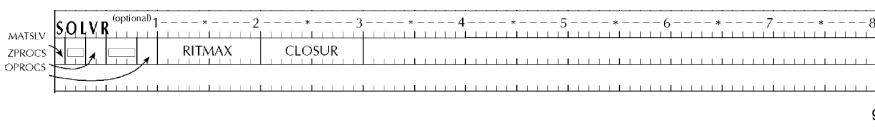
More on Convergence Parameters (PARAM. 3)

- RE1: relative convergence criterion (default: 10^{-5})
$$\left| \frac{R_{n,p+1}^{\kappa,k+1}}{M_{n,p+1}^{\kappa,k+1}} \right| \leq \varepsilon_1$$
- RE2: absolute convergence criterion for ($M < \varepsilon_2$) (default: 1)
$$|R_{n,p+1}^{\kappa,k+1}| \leq \varepsilon_1 \cdot \varepsilon_2$$
- WUP: upstream weighting factor for mobilities and enthalpies (default = 1; recommended)
- WNR: Weighting factor for increments in Newton/Raphson iteration (default = 1; recommended)
- DFAC: increment factor for numerically computing derivatives (default: internally calculated; $\sim 10^{-8}$; check on 64-bit machines and adjust if too low!)

8

Linear Equation Solvers

MOP (21)=0: defaults to MOP (21)=3
 MOP (21)=1: direct solver LUBAND (same as MOP (21)=6)
 MOP (21)=2: DSLUBC, a bi-conjugate gradient solver
 MOP (21)=3: DSLUCS, a Lanczos-type bi-conjugate gradient solver
 MOP (21)=4: DSLUGM, a generalized minimum residual solver
 MOP (21)=5: DLUSTB, a stabilized bi-conjugate gradient solver
 MOP (21)=6: direct solver LUBAND
 Use block SOLVR to select preconditioners (ZPROCS and OPROCS),
 maximum number of iterations (RITMAX),
 and convergence criterion for iterative solvers (CLOSUR)



9

Output Options

Variable	Description	Default
KDATA	Specify amount / type of printout (EOS-specific)	1
	1: Output referring to elements 2: 1 + output referring to connections 3: 2 + primary variables, relative permeabilities	
MCYPR	Printout occurs for every multiple of MCYPR steps	1
MOP (1)	Create printout for non-convergent iterations	no
MOP (7)	Printout of input data (recommended)	no
MOP (2–6)	Additional printout for debugging (→ huge file!)	no

Additional printout times to be specified in block TIMES

```
MOP (i,i=1,24)
PARAM----1-----123456789012345678901234-----5-----6-----7
 8 2 100      5100000100000000400003000
          0.0    86400.0      1.0     3600.0      9.81      4.0
          1.000E-05   1.0          1.0      1.0     1.0E-8
          1.0E+05    10.35        10.35    20.0
```

10

Other MOPS (pp.163-167)

Variable	Description	Default
MOP (9)	Composition of MASS generated fluid	mobility
MOP (10)	Heat conductivity model	sqrt(S_i)
MOP (11)	Weighting scheme (see following 2 slides)	upstream
MOP (12)	Interpolation for time dependent generation	linear
MOP (15)	Semi-analytical heat exchange model	off
MOP (18)	Weighting of interface density	upstream
MOP (19)	Conversion of primary variables (from INCON)	off
MOP (21)	Linear equation solver (see also SOLVR)	DSLUCS
MOP (24)	Weighting of diffusive fluxes	harmonic

```

MOP
PARAM----1-----123456789012345678901234-----5-----6-----7
 8 2 100      510000010000000004000003000
    0.0   86400.0      1.0     3600.0      9.81      4.0
 1.000E-05      1.0      1.0      1.0      1.0E-8
    1.0E+05      10.35      20.0

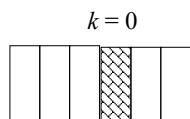
```

11

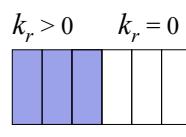
Evaluation of Interface Terms

$$F_{nm}^\kappa = \left[\sum_\beta X_\beta^\kappa \cdot k_{nm} \left(\frac{k_{r\beta} \cdot \rho_\beta}{\mu_\beta} \right)_{nm} \cdot \left(\frac{P_{\beta m} - P_{\beta n}}{d_{nm}} + \rho_{\beta nm} \cdot g \cdot \cos \gamma_{nm} \right) \right]$$

- k , $k_{r\beta}$, ρ_β , μ_β , need to be evaluated at interface nm
- How to average?
 - Harmonic mean for k
 - Upstream weighting for mobility k/μ :
 - Arithmetic mean for ρ



$$k_{i-1/2} = \frac{2k_{i-1}k_i}{k_{i-1} + k_i}$$



$$k_{r,i-1/2} = k_{r,i-1}$$

12

MOP(11)

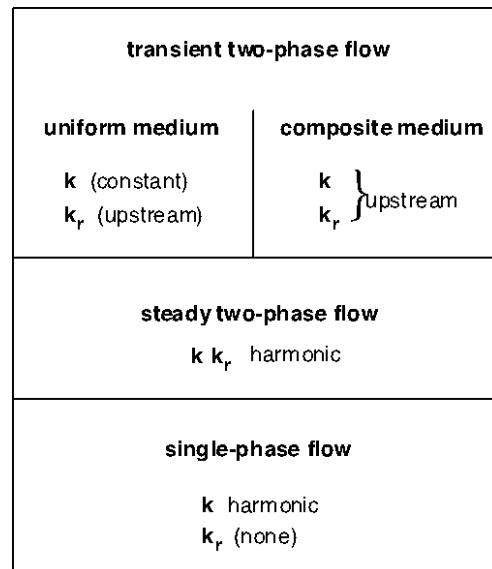
MOP (11)=0: (default)
mobilities upstream;
perm. upstream

MOP (11)=1:
mobilities averaged;
perm. upstream

MOP (11)=2:
mobilities upstream;
perm. harmonic

MOP (11)=3:
mobilities averaged;
perm. harmonic

MOP (11)=4:
mobilities harmonic;
perm. harmonic



13

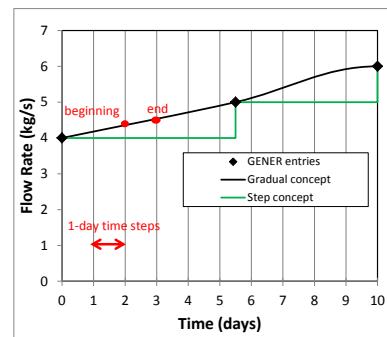
MOP (12) : Time-Dependent Injection/Production Rates

MOP (12):

0: **Triple linear interpolation**; tabular data are used to obtain interpolated rates and enthalpies for the **beginning and end** of the time step; the average of these values is then used.

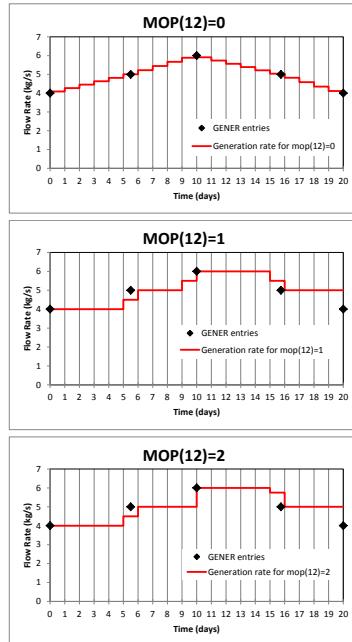
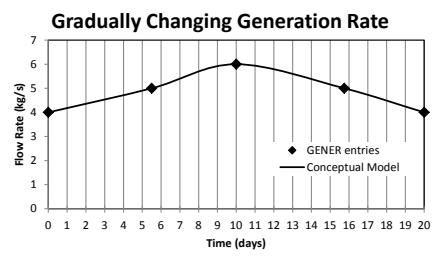
1: **Step function option**; rates and enthalpies are taken as averages of the table values corresponding to the **beginning and end** of the time step.

2: **Rigorous step rate capability**; Tabular data interpreted as **piecewise constant**. Conservation of mass ensured.



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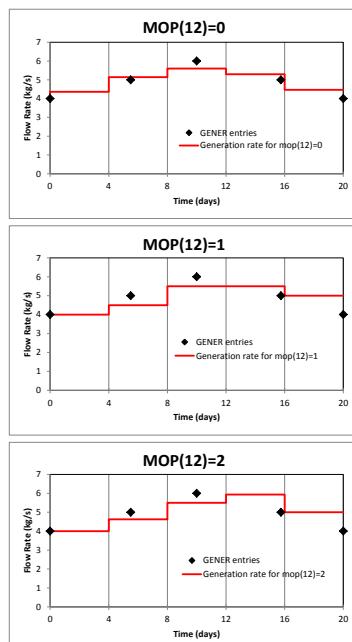
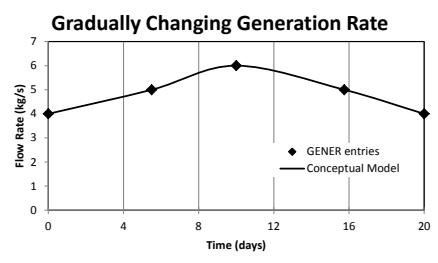
Variable Generation Rate - Example 1



- Gradually changing generation rate
- 1-day time step is short compared to changes in GENER
- $MOP(12) = 0$ recommended

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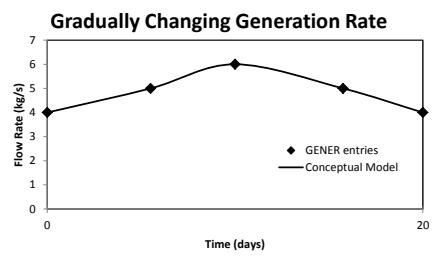
Variable Generation Rate - Example 2



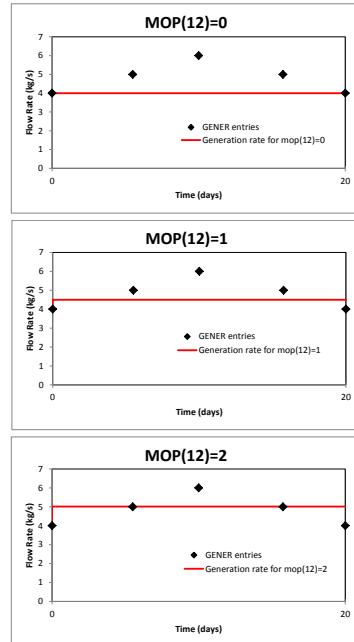
- Gradually changing generation rate
- 4-day time step is comparable to changes in GENER
- Not much difference between $MOP(12)$ choices; $MOP(12)=0$ is best

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Variable Generation Rate - Example 3

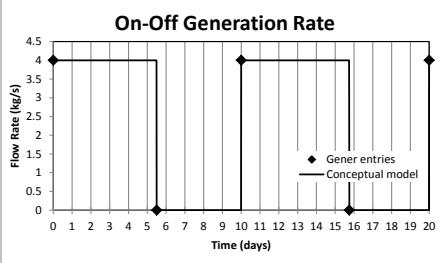


- Gradually changing generation rate
- 20-day time step is long compared to changes in GENER
- MOP(12) = 2 recommended

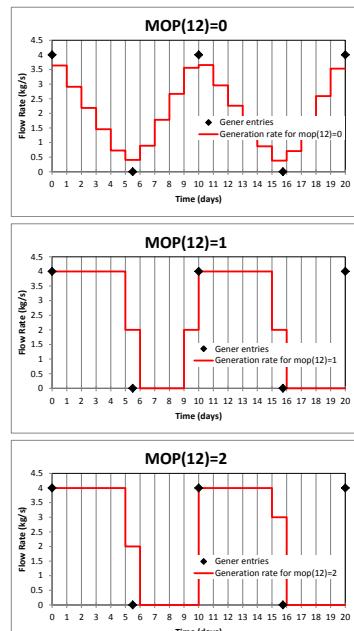


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Variable Generation Rate – Example 4

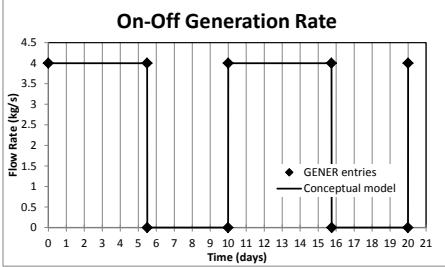


- On-Off generation rate
- 1-day time step is short compared to changes in GENER
- MOP(12) = 2 recommended

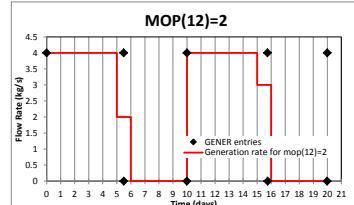
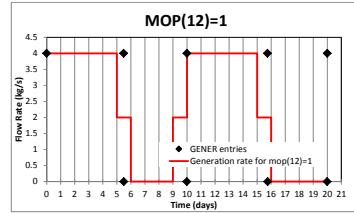
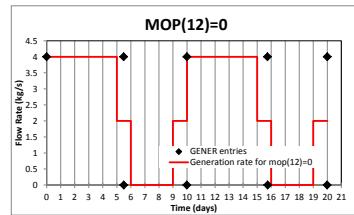


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Variable Generation Rate – Example 5



- On-Off generation rate with extra GENER entries to define steps
- 1-day time step is short compared to changes in GENER
- Not much difference between MOP (12) choices; MOP (12)=2 best



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Why Did TOUGH2 Stop???

- Reached *user-specified* stopping criterion
 - Maximum number of time steps (`MCYC`)
 - Maximum simulation time (`TIMAX`)

20

Why Did TOUGH2 Stop???

- Stops prematurely → Convergence failure
 - Erroneous data initialization → Unphysical primary variables
 - Too many (>10) consecutive time steps converging within a single Newton-Raphson iteration
 - Steady state is reached
 - Time step is too small (check DELTEN, DELTMX, TIMES block)
 - Newton-Raphson error criterion is not tight enough (reduce RE1)
 - Convergence failure following two steps that converged in a single Newton-Raphson iteration
 - May indicate steady state (check whether it actually is!)
 - Serious convergence difficulty (usually phase changes)
 - More than 20 time-step reductions
 - Check initial time step size and initial conditions
 - Check whether simulation time exceeds last GENER time
 - Check for non-monotonous times in block TIMES

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Exercise 1d

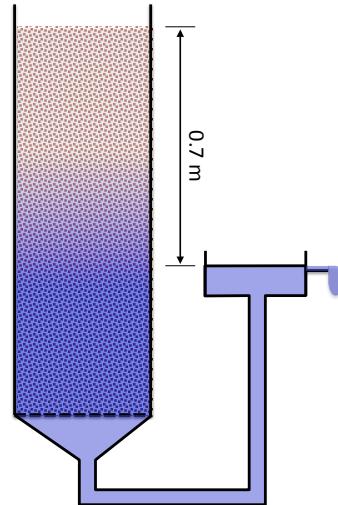
- ✓ Mesh Generation
- ✓ Rock Properties
- ✓ Initial and Boundary Conditions
- Computational Parameters

22

11

Drainage Experiment

- Open file *P1d.txt*
- Edit file so you can simulate the lowering of the water table to a level 0.3 m above the bottom of the column:
 - Use hydrostatic profile from exercise 1c as initial conditions
 - Adjust boundary conditions as needed
 - Provide computational parameters and program options where indicated (“?”)



23

Questions

Q1: Describe the modifications you made to file *P1d.txt* to simulate the drainage of the column.

24

Questions

Q2: What are the liquid and capillary pressure profiles if the drainage experiment were run to steady-state conditions?

Q3: What is the saturation profile above the water table at steady state?

Q4: Confirm your answers to Q2 and Q3 by running the experiment to steady state.

25

Explore TOUGH!

- Perform sensitivity analyses and explore program options. For example:
 - Provide infiltration flux at top
 - Change soil hydraulic properties
 - Make system heterogeneous
 - Change convergence criteria
 - Change weighting schemes
 - Add a gas phase and/or heat (switch to EOS3!)
 - Explore!!!

26



Fractured Rocks

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

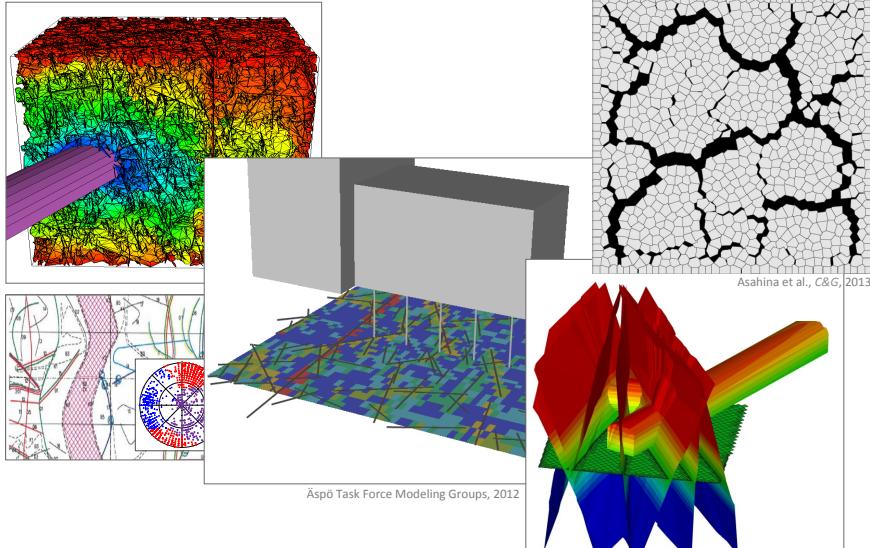
Outline

- Overview
- Discrete fracture network models
- Equivalent continuum model
- Double-porosity model
- Dual-permeability model
- MINC model

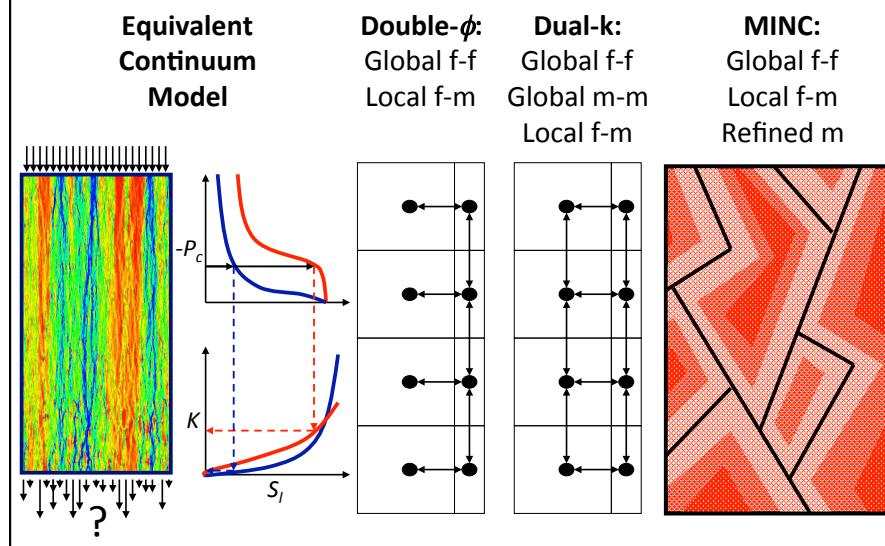
2

1

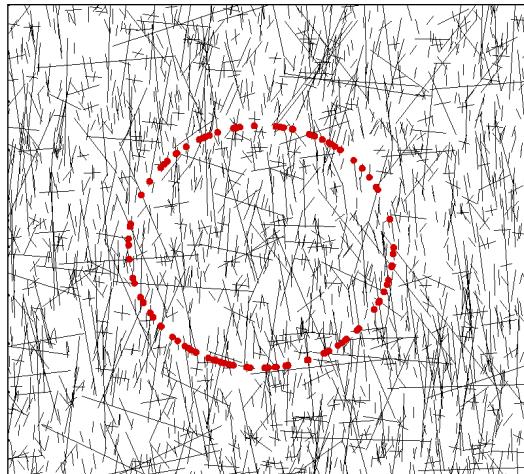
Discretely different fracture models ...



... or multiple-continua models



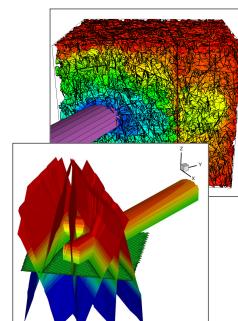
Fractured Porous Media



5

Fractured Porous Media

- Flow characteristics
 - Global, fast flow through fractures
 - Local, slow exchange between fracture and matrix
- Modeling approaches
 - Discrete fracture network model (DFNM)
 - explicit incorporation of individual fractures
 - Continuum approaches
 - effective continuum model (ECM)
 - double porosity model (DPM)
 - dual permeability (DKM)
 - multiple interacting continua (MINC)
 - Combination of discrete and continuum approach
- See Doughty, *J. Contam. Hydr.*, 38, 69-106, 1999

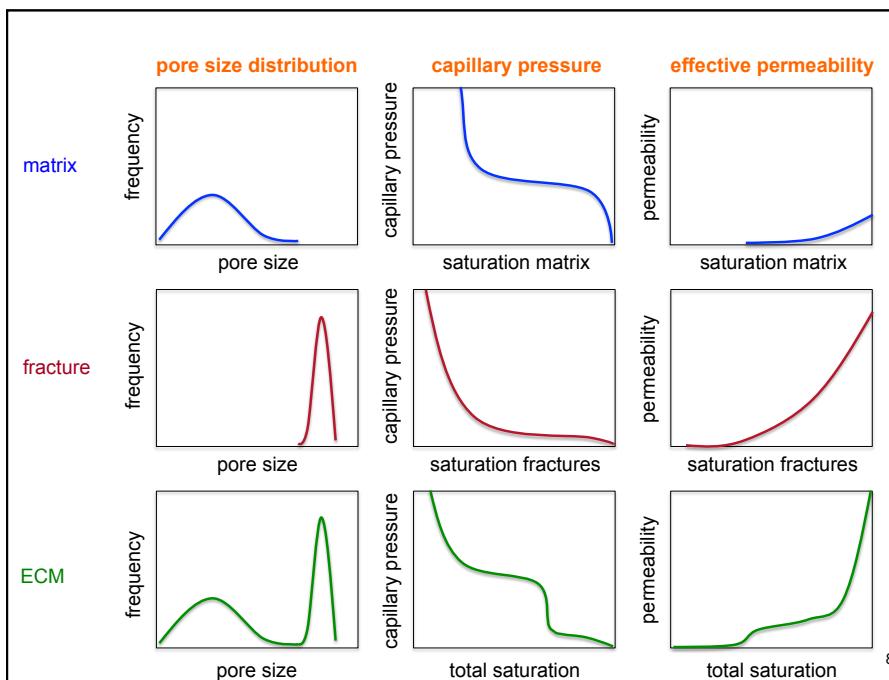


6

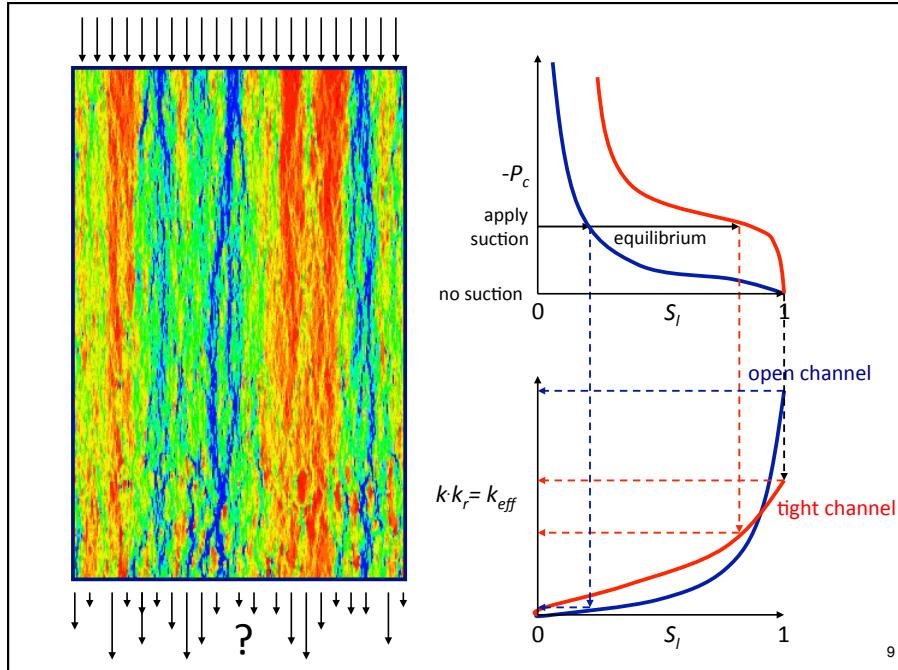
Effective Continuum Model

- Assume **equilibrium** between fracture and matrix continua
- Define a **single, effective continuum** for fractures and matrix
- Use **effective relative permeability and capillary pressure curves** from bi-modal pore-size-distribution model
- (Special TOUGH2 module)

7

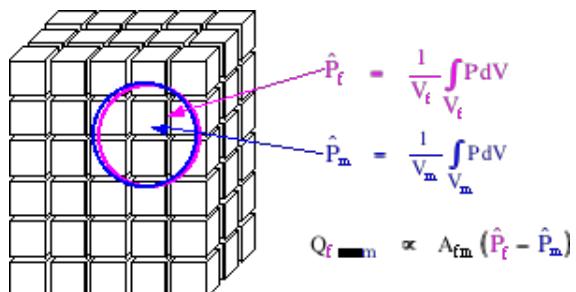


8



Double Porosity

- Two overlapping *continua* (one representing all fractures, the other all matrix blocks)
- Two computational points at each location
- Local interaction between the two continua
- Gridding is *independent* of fracture spacing (gridding needed for numerical solution of *continuum* equations – not to represent fractures!)

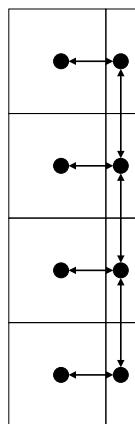


10

Double Porosity/Dual Permeability

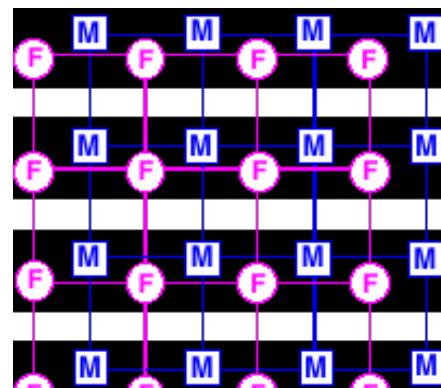
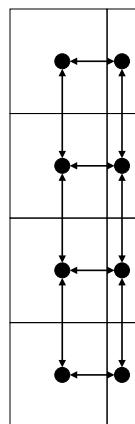
Double- ϕ

Global f-f
Local f-m



Dual-permeability

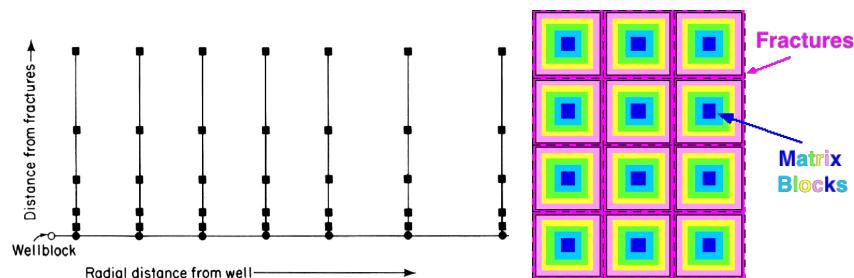
Global f-f
Global m-m
Local f-m



11

Multiple Interacting Continua (MINC)

- Gradient within matrix blocks better resolved through subgridding of matrix into multiple grid-blocks
- Onion-like subgridding as a function of distance from fracture
- Conceptually, global matrix-matrix flow is *not* possible



12

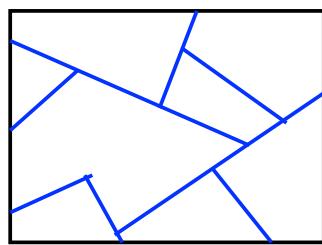
MINC

- Local thermodynamic equilibrium
- Changes in thermodynamic conditions depend on distance from fracture
- Flow essentially perpendicular to fracture faces
- Partition matrix into sequence of nested volume elements, which are defined on the basis of distance from the fractures (see next slide)
- Proximity function $V(x)$ (see next slide)
- Gridding does *not* need to coincide with fracture spacing

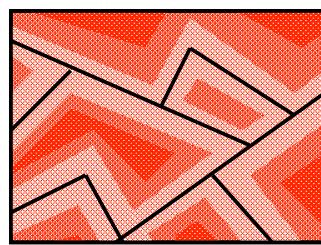
13

MINC Proximity Function

1 fracture continuum



3 nested matrix continua



$$\omega(x) = \frac{V(x)}{V_m} = \frac{V(x)}{(1 - \varphi_1)V_0}$$

$$A(x) = \frac{dV}{dx} = (1 - \varphi_1)V_0 \frac{d\omega(x)}{dx}$$

- All matrix material within a certain distance interval from the fractures is lumped into a continuum and connected to its neighboring shells (either fracture continuum or next matrix continuum)
- Analytical expressions available for regular (and random) fracture networks
- Other, network-specific proximity functions can be defined

14

MINC it in TOUGH!

```
ELEM-----1-----*-----2-----*-----3-----*-----4-----*-----5  
...  
CONNE  
...  
MESHM-----1-----*-----2-----*-----3-----*-----4-----*-----5  
MINC  
PARTTHRED      MMALL  
    5   4OUT      50.0      100.0  
        0.02      0.08      0.20      0.30  
  
ENDCY-----1-----*-----2-----*-----3-----*-----4-----*-----5
```

}

primary MESH

- Two-continua mesh is on file *MINC*
- Fracture elements have element names with a blank first character
- Check normalized volumes, areas, and distances in output file
- Nodal distance from fracture to (first) matrix continuum is zero to ensure that matrix permeability is taken, overwriting upstream-weighting scheme

15

From one Continuum to Two Continua

```
ROCKS-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8  
POMED      2650.      0.02      6.E-15      6.E-15      6.E-15      2.1      1000.  
FRACT      2650.      0.50      6.E-15      6.E-15      6.E-15      2.1      1000.  
MATRX      2650.      0.01      1.E-18      1.E-18      1.E-18      2.1      1000.
```

- The single-continuum properties (**POMED**) in the primary mesh are replaced by two materials, one for the fracture (**FRACT**) and one for the matrix (**MATRX**) continuum
- Check rock type number assigned to elements in file *MINC*
- Total fracture porosity is the product of fracture continuum porosity and fracture fraction

16

Recommended Numerical Methods for Flow in a Fractured Vadose Zone

	Steady Moisture Flow	Transient Moisture Flow	Transient Gas Flow	Tracer Transport*	Thermal Loading**
Matrix only	No	No	No	No	No
Fractures only	No	No	No	No	No
ECM	Yes	Maybe, for large F-M interface area and low flow rate	Yes	Maybe, for large F-M interface area and low flow rate	No
Double porosity	Yes	No	Yes		
Dual permeability	Yes	No	Yes	Maybe, for large F-M interface area and low flow rate	Maybe
MINC	Yes	Yes	Yes	Yes	Yes

*with steady moisture flow

**may induce transient moisture flow

Based on numerical modeling of flow and transport through fractured welded and non-welded tuffs at Yucca Mountain, Nevada (Doughty, *J. Contam. Hydr.*, 38, 69-106, 1999)



Semi-Analytical Heat Exchange

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Semi-Analytical Heat Exchange

1. Heat Exchange with Confining Beds
2. Heat Exchange between Well and Surrounding Formation
3. Exercise

2

1

1. Heat Exchange with Confining Beds

- Modeling heat exchange between reservoir fluids and confining beds possible by extending the computational grid into low-permeability cap-rock and base-rock
 - Heat exchange treated same as flow in the reservoir
 - Requires large number of grid blocks (=inefficient!)
- Semi-analytical method (Vinsome and Westerveld, 1980) implemented in TOUGH2 provides
 - Increased efficiency since no grid blocks outside of fluid flow domain are required
 - Better accuracy for short- and long-term heat exchange

3

Vinsome and Westerveld (1980)

- Since heat conduction tends to dampen out temperature variations, cap- and base-rock temperatures are assumed to vary smoothly even for strong and rapid temperature changes at boundary of conduction zone.
- Assuming that heat conduction perpendicular to the conductive boundary is more important than parallel to it, the temperature profile $T(x,t)$ is represented in a semi-infinite conductive layer by a simple trial function.

4

Vinsome and Westerveld (1980)

$$T(x,t) - T_i = \left(T_f - T_i + px + qx^2 \right) \exp(-x/d)$$

5

Annotations:

- $T(x,t) - T_i$: T at reservoir boundary
- $T_f - T_i + px + qx^2$: Fit parameters
- $d = \sqrt{\Theta t}/2$: Distance from boundary
- $\Theta = \lambda/\rho C$: Specific heat
- λ : Thermal conductivity
- ρ : Density
- C : Thermal diffusivity
- T_i : Initial T (uniform) in cap/base-rock

Implementation in TOUGH2

- Each grid block in the top and bottom layers of the computational grid will have an associated temperature profile in the adjacent impermeable rock as given by $T(x,t)$.
- The coefficients p and q will be different for each grid block; they are determined concurrently with the flow simulation from the physical constraints of (1) continuity of heat flux across the boundary, and (2) energy conservation for the reservoir/confining layer system.

6

Implementation in TOUGH2

To activate semi-analytical heat exchange, a number of parameters have to be specified in different blocks to engage this option, as follows:

- Parameter MOP(15) in record PARAM. 1 is set to 1.
- Initial temperature as well as heat capacity and conductivity of the confining beds are specified by means of data provided for the very last volume element in data block ELEME.
- The initial temperature is taken as the temperature with which the last element is initialized.

7

Implementation in TOUGH2

- Heat capacity and conductivity are taken from data provided in block ROCKS for the particular domain to which the last element belongs.
- Thus, the user appends an additional inactive element in block ELEME, and provides the desired parameters as initial conditions and domain data, respectively, for this element.
- Finally, specify which elements have an interface area with the confining beds, and give the magnitude of this interface area. This information is input as parameter AHTX in columns 31-40 of volume element data in block ELEME. Volume elements for which a zero-interface area is specified will not be subject to heat exchange.

8

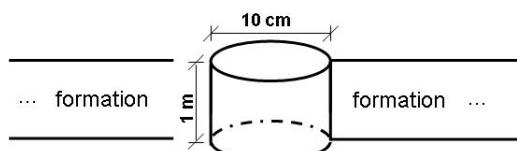
Implementation in TOUGH2

- At the termination of a run the data necessary for continuing the heat exchange calculation in a TOUGH2 continuation run are written onto a disk file TABLE.
- When restarting a problem, this file has to be provided under the name TABLE. If file TABLE is absent, TOUGH2 assumes that no prior heat exchange with confining beds has taken place, and takes their temperatures to be uniform and equal to the temperature of the very last volume element in block ELEM.
- Application of semi-analytical heat exchange is given in sample problem 3 of the TOUGH2 manual (Heat Sweep in a Vertical Fracture).

9

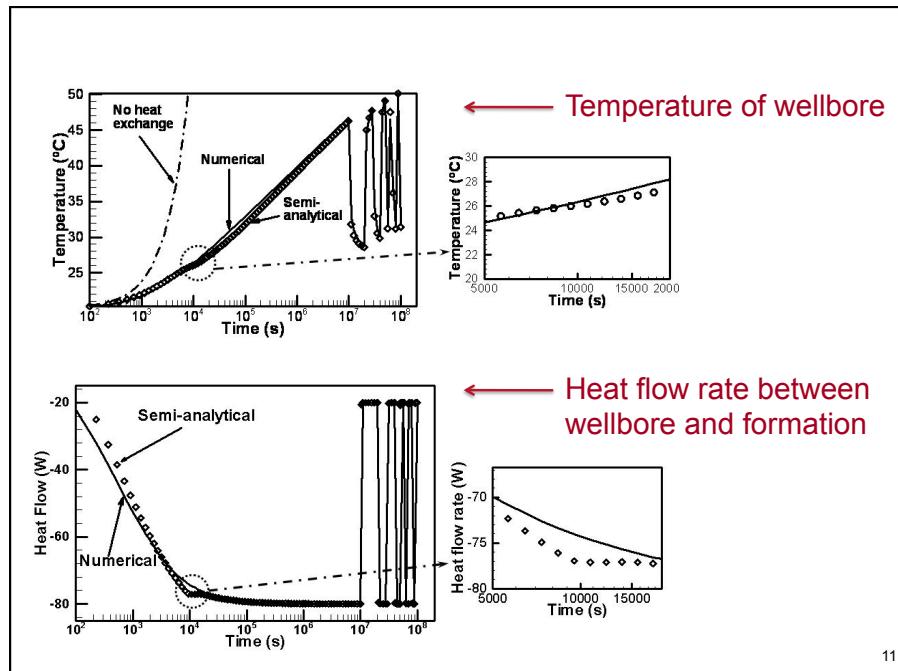
2. Heat Exchange between Well and Surrounding Formation

- Time-convolution approach recently developed (Zhang et al., 2011, *Geothermics*, 40, 261-266)
- Example compares heat injection into a wellbore with (1) semi-analytical solution for, (2) full numerical solution for, and (3) without radial heat conduction



Schematic of wellbore model

10



11

3. Exercise

- What are the reasons for including semi-analytical heat exchange in TOUGH2 simulations?
- Describe the steps necessary to implement semi-analytical heat exchange between reservoir fluids and a confining layer.

12



Phase Change

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Objectives

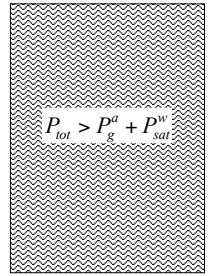
- Understand thermodynamics of two-phase, two-component system (EOS3)
- Understand primary variables, phase state, problem initiation, and variable switching

2

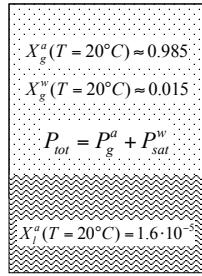
1

Phase State and Primary Variables

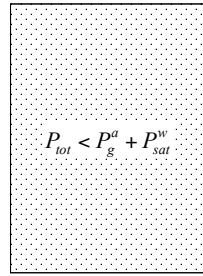
Mass fraction: $X_\beta^\kappa = \frac{m_\beta^\kappa}{m_\beta} = \frac{m_\beta^\kappa}{\sum_{\kappa=1}^{NK} m_\beta^\kappa} = \frac{x_\beta^\kappa M^\kappa}{\sum_{\kappa=1}^{NK} x_\beta^\kappa M^\kappa}$ $\sum_{\kappa=1}^{NK} X_\beta^\kappa = 1$ $M^\kappa = m^\kappa / n$



Single-phase liquid
 P_g, X_l^a, T



Two-phase gas-liquid
 $P_g, 10+S_g, T$



Single-phase gas
 P_g, X_g^a, T

3

EOS3

Q1: Which phases and components does EOS3 handle?

Phases: _____

Components: _____

Q2: What are the primary variables for single-phase conditions?

Q3: What are the primary variables for two-phase conditions?

4

EOS Primary Variables

Q4: Why is 10 added to the second primary variable for two-phase conditions?

Q5: How can you tell from the primary variables whether a grid block is single-phase liquid or single-phase gas?

5

EOS3 Primary Variables (cont.)

Q6: What is the phase state of a grid block with the following primary variables?

1.013E+5 0.2 20.0

Q7: Provide the second primary variable for a grid block at 50% relative humidity?

1.013E+5 ??? 20.0

6

EOS3 – (non)isothermal

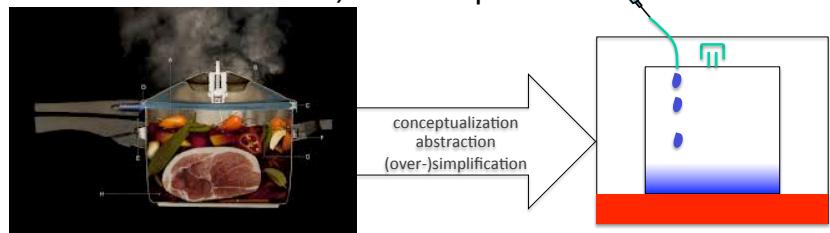
Q8: How do you tell TOUGH2 that a simulation should be isothermal or nonisothermal?

Q9: Why do you need to specify a temperature for each grid block even if you perform an isothermal simulation?

7

Phase Change - Yes, We Can!

- Simulate an (almost) tight *pressure cooker*...
- ...represented by only two grid blocks!
- Discuss each block of input file shown on following slide (specifically initial conditions)
- *Before* running the simulation, predict thermodynamic state in each grid block
- Run simulation; answer questions



8

```

Demonstration of phase changes
ROCKS----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
POT      0       2720.0      0.90     1.0E-17          81.0      1000.0
KITCH    0       1.0E30      0.05     1.0E-17          81.0     100000.0

RPCAP----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
 1           0.00      0.99      1.0       1.0
 1           0.0       0.10      1.0
MULTI----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
 2       3       2       6
PARAM----1---MOP:123456789012345678901234----5-----6-----7-----*-----8
 8 1 100      100100030100001000400003000
 0.000E+00   3.600E+03    -1.0   1.000E+02
 1.0E-7     0.999999      9.0      90.0
 1.000E-06
               1.0E5      10.995      20.0

ELEME----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
POT 1        1       1.0E-3
KIT 2        2       1.0E+4

CONN-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
POT 1 KIT 2      1       0.05     0.0001      0.01

START----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
INCON----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
KIT 2
               1.0E+5      1.0       200.0

GENER----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
POT 1WAT 1      6       WATEr      1.00     8.39E+4
 0.0      1300.0      1301.0      1500.0
 1501.0    1.0E50
 0.0       0.0       4.5E-3      4.5E-3
 0.0       0.0
 8.39E+4    8.39E+4      8.39E+4      8.39E+4
 8.39E+4    8.39E+4

TIMES----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
 6
 1.0E-6     1300.0      1301.0      1400.0      1500.0      3600.0

ENDCY----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8

```

9

Phase Change

Q10: Describe simulated experiment

10

Phase Change

Q11: How much liquid water (in liters) is in the pot?

Q12: What phase state do you expect at:

0 sec: _____

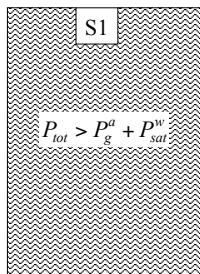
1300 sec: _____

1500 sec: _____

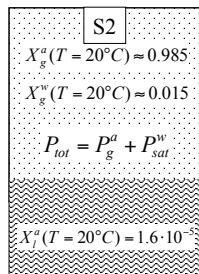
3600 sec: _____

Run the simulation now!

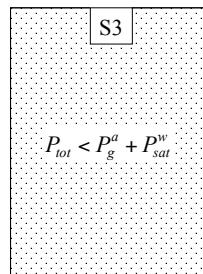
11



Single-phase liquid
 P_g, X_l^a, T



Two-phase gas-liquid
 $P_g, 10+S_g, T$



Single-phase gas
 P_g, X_g^a, T

Time 0~1300 s, S2 → S3 by ↑ T

Time 1301~1500 s, S3 → S2 → S1 by injecting liq., ↑ P, ↓ S_g

Time 1501~3600 s, S1 → S2 by ↑ T

12

Q13: Check the volume of liquid in the pot;
compare to your answer to Q11.

Q14: How much water vapor is initially in the pot?

Q15: How much water vapor is in the pot at
 $t=1300$ sec?

13

Q16: How is heat added to the pot?

Q17: Why is the pressure so high after 1500 s?

Q18: What is the final phase state (at $t=3600$ s)
and why?

14

Q19: Change the input file and remove the “safety valve” (or vent). What do you expect to happen and when? Rerun the simulation and describe the result.

15



Radionuclide Transport

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California

1

Objectives

- Understand transport of decaying radionuclides under non-isothermal two-phase flow conditions
- Learn about TOUGH2 module EOS7R

2

1

EOS7R At a Glance

- Components

1. Water
2. Brine
3. Air
4. Radionuclide 1 (“parent”)
5. Radionuclide 2 (“daughter”)
6. Heat

- Phases

1. Gas
2. Liquid
 - (no salt precipitation)

- Radionuclide-related processes

- Decay
- Radionuclides are water soluble and volatile
- Sorption to solids (Kd approach)
- Molecular diffusion in liquid and gas phases

3

Brine

- Brine properties modeled as a function of reference brine mass fraction X_b .
- Density of aqueous mixtures of brine and water: Fluid volume is conserved:

$$\frac{1}{\rho_m} = \frac{1 - X_b}{\rho_w} + \frac{X_b}{\rho_b}$$

- Mixture viscosity as a function of P , T , and X_b :

$$\begin{aligned}\mu_m(P, T, X_b) &= \mu_w(P, T) \cdot f(X_b) \\ f(X_b) &= 1 + \nu_1 X_b + \nu_2 X_b^2 + \nu_3 X_b^3\end{aligned}$$

- Default reference brine (24.98 wt% NaCl; 5.06 molar)

$$\begin{aligned}\rho_b(P = 10^5, T = 25, X_b = 1) &= 1183.1 \text{ kg/m}^3 \\ f(X_b) &= 1 + 0.4819 X_b - 0.2774 X_b^2 + 0.7814 X_b^3\end{aligned}$$

4

Radioactive Decay

- Exponential decay of mass (M) of radionuclide k

$$\frac{dM^k}{dt} = -\lambda_k M^k$$
$$M^k = M_0^k \exp(-\lambda_k t)$$

- Half-life depends on decay constant λ_k

$$\frac{M_{t_{1/2}}^k}{M_{t_0}^k} = \exp(-\lambda_k t_{1/2}) = \frac{1}{2}$$
$$t_{1/2} = \frac{\ln 2}{\lambda_k}$$

5

Sorption and Dissolution of Radionuclides

- Mass adsorbs onto solid grains by reversible instantaneous linear model

$$M^k = \phi \sum_{\beta} S_{\beta} \rho_{\beta} X_{\beta}^k + (1-\phi) \rho_R \rho_{aq} X_{aq}^k K_d$$

- Gas dissolution in the aqueous phase determined by Henry's law

$$P_k = K_h X_{aq}^k \quad \text{or} \quad X_{aq}^k = (K_h^{-1}) P_k$$

6

Primary Variables

Pressure	P
Mass fraction of brine	X_b
Mass fraction of Rn1	X_{Rn1}
Mass fraction of Rn2	X_{Rn2}
Mass fraction of air	X_{air}
Gas phase saturation	S_g
Temperature	T

Single-phase Two-phase

7

Primary Variables

Choice of primary variables (X1-X6) determines phase conditions:

	X1	X2	X3	X4	X5	X6
1-phase (aq.)	P	X_b	X_{Rn1}	X_{Rn2}	X_{air}	T
2-phase (aq. + gas)	P	X_b	X_{Rn1}	X_{Rn2}	$S_g + 10$	T

- Number of unknowns can be reduced in MULTI block
 - If gas is excluded, NK = 4 (NK = 5 otherwise)
 - If INCON from EOS7 run (NKIN = NK - 2)
 - Ignore diffusion: NB = 6; Include diffusion: NB = 8

8

Components

- #1: water
- #2: brine
- #3: Rn1 (radionuclide 1; "parent")
- #4: Rn2 (radionuclide 2; "daughter")
- #5: air (optional)[†]

Parameter choices

(NK, NEQ, NPH, NB) [§] = (5, 5, 2, 8) water, brine, Rn1, Rn2, air, isothermal (default)
(5, 6, 2, 8) water, brine, Rn1, Rn2, air, nonisothermal
(4, 4, 2, 8) water, brine, Rn1, Rn2, no air, isothermal[†]
(4, 5, 2, 8) water, brine, Rn1, Rn2, no air, nonisothermal[†]

molecular diffusion can be suppressed by setting NB = 6

Primary Variables[§]

single-phase conditions
 $(P, X_b, X_{Rn1}, X_{Rn2}, X_{air}, T)$ - (pressure, brine mass fraction, mass fraction of Rn1, mass fraction of Rn2, air mass fraction, temperature)

two-phase conditions
 $(P, X_b, X_{Rn1}, X_{Rn2}, S+10, T)$ - (gas phase pressure, brine mass fraction, mass fraction of Rn1, mass fraction of Rn2, gas saturation plus ten, temperature)*

[†] the no air option ($NK = 4$) may only be used for problems with single-phase liquid conditions throughout

[§] parameter $NKIN$ following NB may optionally be set to $NKIN = NK-2$, in which case radionuclide mass fractions will be omitted, and initialization will be made from only four EOS7-style variables; radionuclide mass fractions will be initialized as zero;

* in two-phase conditions, X_{Rn1} and X_{Rn2} are mass fractions in the aqueous phase

9

SELEC Block

- SELEC block holds **brine** properties and **radionuclide** properties related to decay, diffusion, and solubility

```
SELEC----1-----*----2-----*----3-----*----4-----*----5-----*----6-----*----7-----*----8
      6
Brine reference conditions (P, T, density for Xb = 1.0)
Coefficients for brine viscosity (see Eq. 9)
Dispersivities (T2DM only)
Diffusion coefficients for water, brine, and air (overwritten by DIFFU block)
Properties of Radionuclide 1 (parent)
Properties of Radionuclide 2 (daughter)
```

```
SELEC----1-----*----2-----*----3-----*----4-----*----5-----*----6-----*----7-----*----8
      6          P          T          Rho (compressibility and expansivity same as water)
      1.0E5      25.0      1185.1 (if 0: reference brine as shown; P < 0: like water)
      0.4819     -0.2774     0.7814 (if 0: default values as shown)
      v1          v2          v3 (see Eq. 9)

      1.44e+10    241.0     1.e-6   1.162e-9          1.e+30
      6.0e+13     237.0     1.e-6   1.162e-9          1.e+30
half-life       Mw          Dg          Dl          Henry
      [s]        [g/mol]    [m^2/s]    [m^2/s]    [Pa^-1]
```

10

ROCKS Block (Adsorption)

- Material-specific distribution coefficients, K_d [m³/kg], for radionuclides in aqueous phase

$$M^k = \phi \sum_{\beta} S_{\beta} \rho_{\beta} X_{\beta}^k + (1 - \phi) \rho_R \rho_{aq} X_{aq}^k K_d$$

ROCKS-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8								
MAT	NAD	DROK	POR	PER(1)	PER(2)	PER(3)	CWET	SPHT
COM	EXPAN	CDRY	TORTX	GK	XKD3	XKD4		
IRP		RP(1)	RP(2)	RP(3)	RP(4)	RP(5)	RP(6)	RP(7)
ICP		CP(1)	CP(2)	CP(3)	CP(4)	CP(5)	CP(6)	CP(7)

ROCKS-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8								
CLAY	2	2650.	.12	1.00E-17	1.00E-17	1.00E-17	2.5	905.5
	$1.83e-9$	$3.47e-5$		1.		$1.00e-00$	$1.00e-03$	
	7	0.4	0.5	1.0	0.05			
	7	0.4	0.5	$5.6e-7$		1.0		

11

EOS7R Sample Problem

Problem description

Part A: Material properties

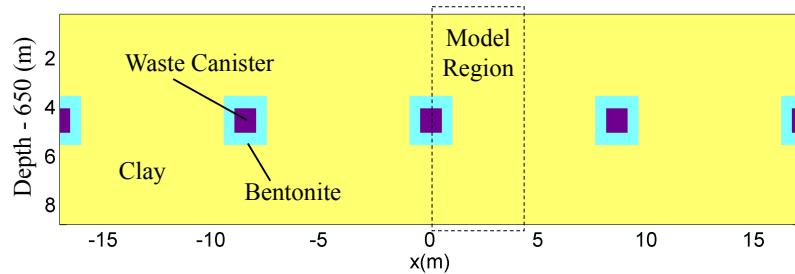
Part B: Mesh generation

Part C: Initial conditions

Part D: Radionuclide Case 1

Part E: Radionuclide Case 2

Problem Description

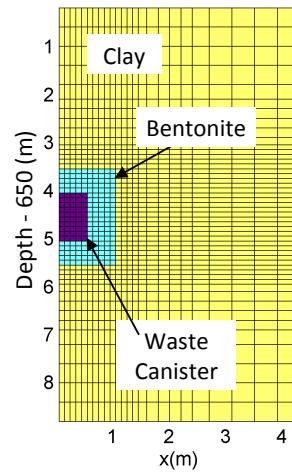


- Case 1: Release of ^{241}Am and decay into ^{237}Np
Aqueous phase, isothermal
- Case 2: Generation of ^{14}C and decay into nitrogen gas
Two-phase, nonisothermal

13

Model

- Two-dimensional model takes advantage of symmetry
 - Irregular grid spacing
- Initial Conditions
 - Single-phase aqueous
 - Flow in vertical direction (downward)
- Boundary conditions
 - Constant conditions at top
 - Constant conditions at bottom (zero flux during static equilibration)
 - Zero flux at the sides



14

Part A: Material Properties

```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS---1-----2-----3-----4-----5-----6-----7-----8
CLAY    2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5   905.5
        1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
        7       0.4       0.5       1.0       0.05
        7       0.4       0.5       5.6e-7          1.0
CONTA   2      2650.     .17   1.00E-17  1.00E-17  1.00E-17   52.0   905.5
        1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
        7       0.4       0.3       1.          0.05
        7       0.4       0.3       1.E-5          1.0
BENTO   2      2650.     .40   1.00E-20  1.00E-20  1.00E-20   1.35   964.0
        3.58e-9  1.5e-5          1.          1.00e-00  1.00E-03
        7       0.4       0.3       1.          0.05
        7       0.4       0.3       5.6e-9          1.0
TOPBC  2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5   905.5
        1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
        7       0.4       0.5       1.          0.05
        7       0.4       0.5       5.6e-7          1.0
BOTBC  2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5   905.5
        1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
        7       0.4       0.5       1.          0.05
        7       0.4       0.5       5.6e-7          1.0
```

Portion of input file *MatDist.txt* containing entries in ROCKS block for three materials: Clay (CLAY), Bentonite (BENTO) and the waste container (CONTA). Two additional materials (TOPBC, BOTBC; with same properties as clay) can be used as boundary materials.

15

Q-A.1: (a) Which material has the lowest permeability, and (b) is the permeability modeled as isotropic or anisotropic?

(a) _____

(b) _____

Q-A.2: What functions are being used to model the relative permeability and capillary pressure?

Q-A.3: How does the capillary pressure behavior for the bentonite buffer differ from that for the waste canister and clay materials?
(Hint: look at CP(3))

16

Part B: Mesh Generation

B.1 Generate 1-D mesh in x-direction

- Open *MakeMesh.txt*
- Fill in correct number of grid increments in the x-direction
- Run code by typing:
`xt2_7r < MakeMesh.txt > MakeMesh.out`
- Open output file *MESH*

Q-B.1.1: What are the minimum and maximum x, y and z values?

17

Q-B.1.2: Calculate the minimum and maximum element volumes from the input file and compare with those generated in the *MESH* file. Do they agree?

Q-B.1.3: In any single connection, the distances from the element centers to the nodes (D1 and D2) may be different. Explain why.

18

Input file *MakeMesh.txt*

```
*RADIONUCLIDE TRANSPORT PROBLEM*
MESHM---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8
XYZ
    0.
NX    ???
    0.1      0.1      0.1      0.1      0.1      0.1      0.1      0.1
    0.1      0.1      0.1      0.1      0.1      0.1      0.1      0.2
    0.2      0.2      0.2      0.2      0.4      0.4      0.4      0.4
    0.4
NY      1      1.0
NZ      1      1.0

ENDFI
*****
Use this distribution of z-direction grid increments to generate 2-D mesh
*****
NZ      5      0.4
NZ      5      0.2
NZ     15      0.1
NZ     15      0.1
NZ      5      0.2
NZ      5      0.4
```

19

B.2 Generate 2-D mesh

- A distribution of z-direction grid increments is given at the bottom of *MakeMesh.txt*. Copy the corresponding lines of text and paste them in the appropriate place in the MESHM block (i.e., replace the line containing "NZ 1 1." with those lines.)
- Note the alternative way to specify grid increments in the z-direction (compared to that used for the x-direction)
- Run code and open output file *MESH*

Q-B.2.1: What are the minimum and maximum x, y and z values?

20

Q-B.2.2: Examine the naming convention for the element names. In this case, how are the five-character element names related to the element coordinates? For example, how can you tell in what column an element is found simply by looking at the element name?

B.3 Assigning material properties to mesh (ELEM block)

➤ Open *MESH_MatNum*. This file is similar to the mesh generated in the previous step except that the material distribution specific to this sample problem has already been generated (material numbers have been inserted in the spaces for parameter MA2 in columns 19-20).

21

Q-B.3.1: Given the material properties specified in *MatDist.txt*, what are the (a) names and (b) depths corresponding to the elements at the top and bottom of the waste container?
(Hint: CONTA is material number 3)

Q-B.3.2: What is the maximum x-coordinate corresponding to the presence of bentonite?

22

Part C: Simulating Initial Conditions

Before simulating radionuclide transport, steady-state conditions under single-phase aqueous flow must be calculated (and then used as initial conditions).

- Open *MatDist.txt* and rename it *SimInit.txt*.
- Copy and paste contents of file *MESH_MatNum* into *SimInit.txt*. Place the contents under the empty INCON block (leaving one blank line in between). Close CONNE block with blank line. Now the input file contains the generated mesh information.
- To obtain steady-state distribution most efficiently, parameters of the MULTI block can be specified to exclude gas from the simulation (NK=4) and to run the code under isothermal conditions (NEQ=4). Make these changes in *SimInit.txt*.

23

Q-C.1: What are the primary variables for this case?

Q-C.2: Given their positions in the input file (PARAM .4 and .5), what are the current initial values of the primary variables?

```
...
MULTI-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
? ? 2 8
START-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
-----*-----1 MOP: 123456789*123456789*1234 -----*-----5-----*-----6-----*-----7-----*-----8
PARAM-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
 39999   99991           4      5           1.0e-1           9.8
 1.E-05    1.E+0           6.37E6          1.0e-3           0.0           0.0
 25.0
...
```

Portion of input file *MatDist.txt*

24

C.1 Creating hydrostatic profile

In order to create a hydrostatic profile, a constant pressure is specified at the upper layer of the model, and a no flow boundary is specified at the bottom of the model.

- The elements at the bottom of the ELEM block correspond to the upper layer of the model (since the MESH was modified). Make this layer inactive by adding a line with “INA” above element “A11 1”. All elements below will become inactive.
- Use the INDOM block to specify the pressure at the upper layer of the model. Copy INDOM block at bottom of file and paste below GENER block (leaving blank line before and after INDOM block).
- Specify the correct material name in INDOM block (i.e., replace ????? with appropriate material name).
- Specify $P = 6.37 \text{ MPa}$ (approximate pressure at 650 meters) and salt mass fraction $X_b = 1.0\text{e-}3$ in the INDOM block.

25

Steady-state conditions are approximated when the primary variables stop changing with increasingly large time steps. For this to occur, the maximum number of time steps to be calculated (MCYC) and the maximum time step (DELTMX) must be large (so that the code does not terminate before reaching steady state). These parameters are modified for time step control and are given in the PARAM block.

Q-C.1.1: What are the values of MCYC, DELTMX and DELTEN?

- Make sure MCYC is a large enough number
- Save input file as *SimInit.txt* and run code

26

Q-C.1.2: What was the maximum simulation time reached? Does this indicate that steady-state conditions were reached? (Open the output file and scroll down to the first occurrence of “OUTPUT DATA”) Confirm your answer by examining *SAVE* file and determining whether the pressure profile changes with depth.

- If steady-state conditions were not reached, the initial time step was probably too small in this case. Change DELTEN to 1.0e+3
- Re-run the code and rename *SAVE* file as *SAVE_SimInit*.

27

Q-C.1.3: Open the main output file (e.g., *SimInit.out*) and examine the results. (a) Is the maximum simulation time indicative of steady-state conditions? Why? (b) How many iterations were completed?

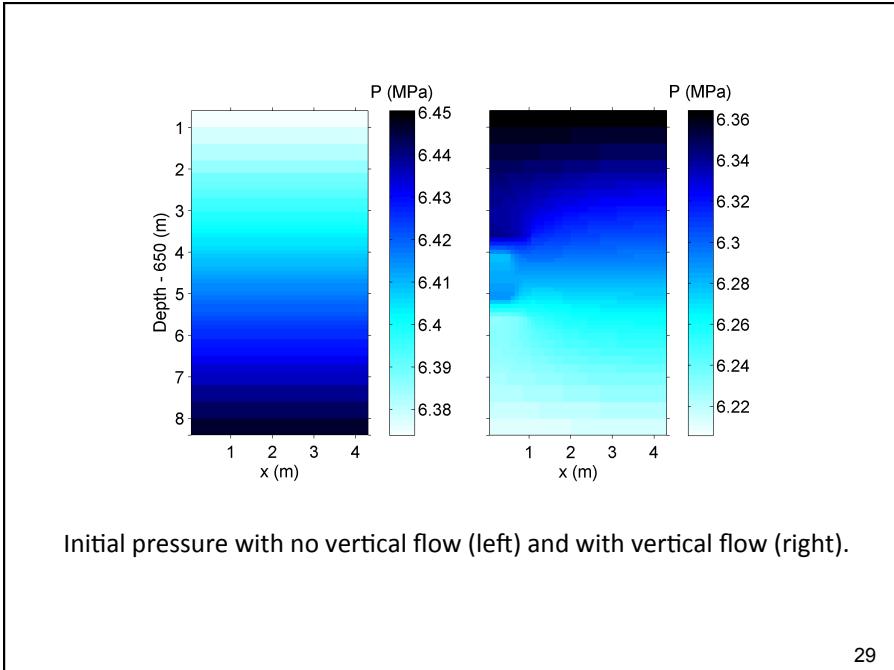
(a) _____

(b) _____

Q-C.1.4: Does the pressure at the bottom of the model match the expected hydrostatic pressure (given the depth of water)?

Q-C.1.5: Determine whether the amounts of water and brine in the system are the same before and after the simulation. Explain why or why not.

28



29

C.2 Creating steady-state profile with vertical flow

In order to induce vertical flow, constant pressures are specified at the upper and bottom layers of the model. For this case, the elements on the top *and* bottom of the model must be made inactive.

- Save `SimInit.txt` as `SimInit_Flow.txt`
- Move the line in the `ELEM` block with “`INA`” to the location right above the element “`BF1 1`” in order to make the upper and lower layers of the model inactive.
- Make the pressure in the lower layer equal to 6.2 MPa. To do this, another modification of the `INDOM` block is needed. In addition to the entry for `TOPBC`, add an entry for the elements at the bottom of the model (`BOTBC`). Be sure to specify the correct material name.
- Save file and run code. Rename resulting `SAVE` file as `SAVE_SimInit_Flow` (it will be used in Part D).

30

Part D: Radionuclide Case 1

In this problem, the release of ^{241}Am and its subsequent decay into ^{237}Np are simulated using the model developed in Parts A-C. The goal is to examine the following:

- Radionuclide release in center of waste container
- Distribution of radionuclides after 2000 years

- Americium 241 (^{241}Am)
 - Among isotopes resulting from weapons production
 - The half life is $t_{1/2} = 458$ years (or $1.44\text{e+}10$ sec)
 - Strongly sorbing, Kd value ~ 1.0 (m^3/kg)
- Neptunium 237 (^{237}Np) is the daughter radionuclide
 - Long-lived decay product of ^{241}Am
 - The half life is $t_{1/2} = 2.14\text{e+}6$ years (or $\sim 6.0\text{e+}13$ sec)
 - Weakly sorbing, Kd value $\sim 1.0\text{e-}3$ (m^3/kg)

31

- Save *SimInit_Flow.txt* and rename it *SimRad1.txt*.
- The file *SAVE_SimInit_Flow* contains the initial conditions that will be used in this simulation. Copy and paste the contents of this file into the main input file (*SimRad1.txt*) in the location of the empty **INCON** block. Only one line with the “**INCON**” keyword should remain. Close the **INCON** block with a blank line. Now the input file contains the needed initial conditions.
- Remove the **INDOM** block
- This case will not involve the evolution of gas, so keep the **MULTI** block the same as the previous one (NK=4 and NEQ=4).

32

D.1 Radionuclide properties

In order to simulate an instantaneous release of ^{241}Am , the parent and daughter radionuclide properties must be specified in the input file as well as the distribution coefficients for each material.

- Add the given half-lives for the parent and daughter radionuclides (Rn1 and Rn2) and the molecular weights

```
...
SELEC----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
   6      1     24      2
   -1.e5

  0.e-0    0.e-1
  0.e-6    0.e-6    0.e-6  1.162e-7    0.e-6    0.e-6
  1.0e1     1.0     0.e-6  1.162e-9
  1.0e1     1.0     0.e-6  1.162e-9
                                         1.e+30
                                         1.e+30
...
...
```

Example of SELEC block from input file.

33

Q-D.1.1: What number is used for the inverse Henry's constant and what does it imply for the assumption of NK = 4 (Hint: is gas formation likely to occur)?

- Check that the correct Kd values are used in the ROCKS blocks (specify XKD3 and XKD4 for each material on lines ROCKS .1 .1).
- Enter maximum simulation time of 2000 years (parameter TIMAX on line PARAM .2). Units must be seconds (6.3072e+10).
- If a line with a “+++” remains in your INCON block, remove it and the following line (but keep blank line after it). This is information from the previous simulation used to track time (e.g., absolute time reached and total number of time steps). Here the previous run was performed to establish steady-state conditions ending at $t=0$, so the continuation info is not needed.

34

D.2 Radionuclide Source

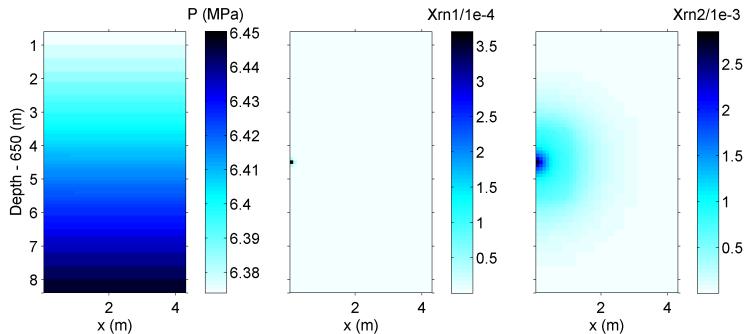
- The third and fourth primary variables (X3 and X4) are the mass fractions of Rn1 and Rn2. Simulate an instantaneous release of ^{241}Am by specifying X3 = 1.0e-3

Q-D.2.1: How could this be made a constant source rather than instantaneous? (Hint: a change in the ELEME block would be required)

```
INCON-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
...
AO1 1          0.17001265E+00
0.6410668430968E+07 0.9999999999942E-03 0.00000000000000E+00 0.00000000000000E+00
0.25000000000000E+02
AP1 1          0.17001296E+00
0.6411648402189E+07 0.1000000000028E-02 1.00000000000000E-03 0.00000000000000E+00
0.25000000000000E+02
AQ1 1          0.17001326E+00
0.6412628373835E+07 0.1000000000024E-02 0.00000000000000E+00 0.00000000000000E+00
0.25000000000000E+02
...
```

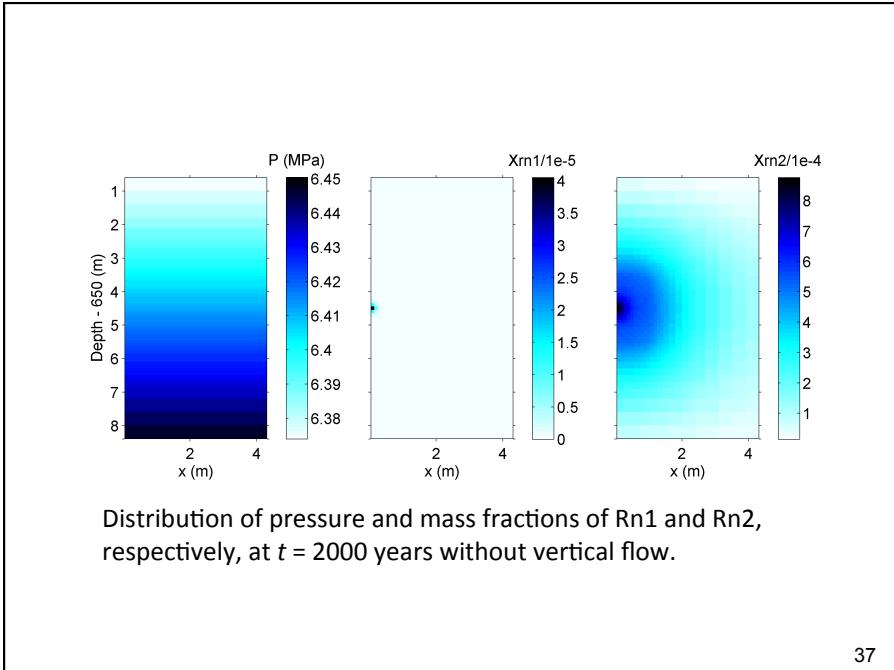
Specifying release of Rn1 in INCON block.

35

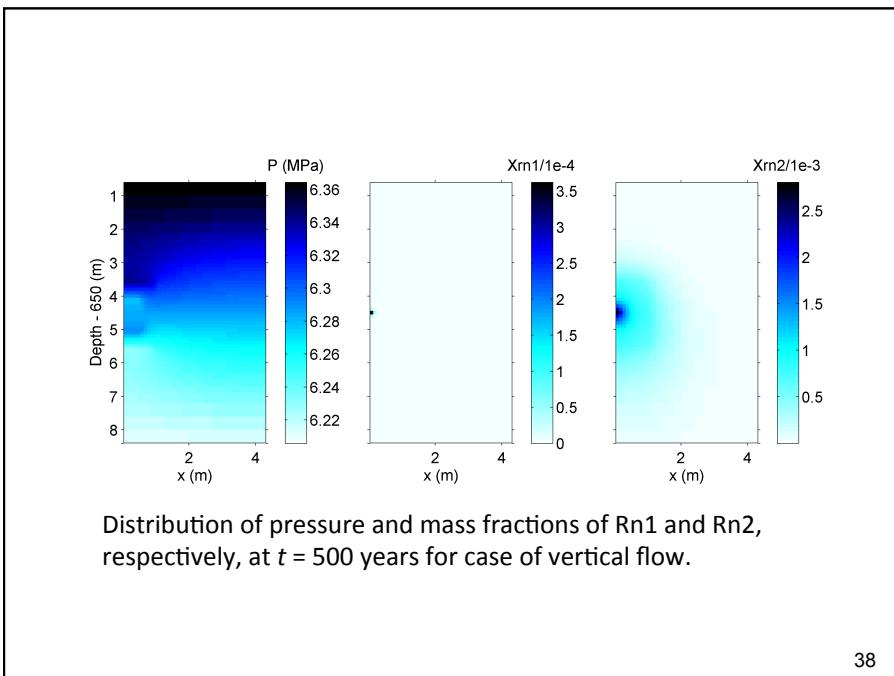


Distribution of pressure and mass fractions of Rn1 and Rn2, respectively, at $t = 500$ years without vertical flow.

36

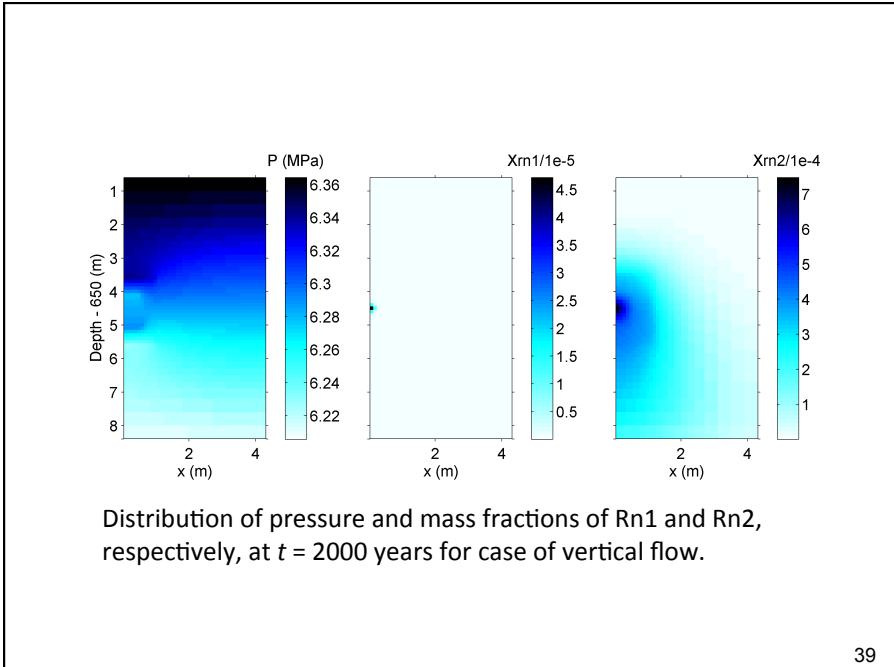


37



38

19



39

Part E: Radionuclide Case 2

A corrosion process is considered in which gas containing carbon 14 (^{14}C) is generated from the waste package along with heat. ^{14}C subsequently decays into nitrogen gas. Pressure build-up within the waste package is examined, along with potential effects on transport of a fracture in the bentonite.

- Carbon 14 (^{14}C)
 - Unstable isotope of carbon ($t_{1/2} = 5730$ years or $1.8\text{e}11$ sec)
 - Contained in activated metals from nuclear reactor components that corrode in the subsurface (slowly releasing ^{14}C)
 - $K_d = 5.0\text{e}-4 \text{ m}^3 \text{ kg}^{-1}$ and $K_H^{-1} = 1\text{E}-8 \text{ Pa}^{-1}$
- Nitrogen 14 (^{14}N) is the daughter product
 - Non-decaying ($t_{1/2}$ is infinite)
 - $K_d = 5.0\text{e}-4 \text{ m}^3 \text{ kg}^{-1}$ (assumed) and $K_H^{-1} = 1\text{E}-10 \text{ Pa}^{-1}$

40

20

➤ Open file *SimRad2.txt*

➤ Modify the **MULTI** block to allow for gas phase and heat to be included in the simulations (NK=5 and NEQ=6).

Q-E.1: The initial conditions were already generated for this simulation. Explain the main difference between the initial conditions in this file (look in **INCON** block) and those generated for the hydrostatic conditions in section Part C.1 (look at file *SAVE_SimInit*).

Q-E.2: Based on the **INCON** block, what is the initial gas saturation in the system?

41

```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS---1-----2-----3-----4-----5-----6-----7-----8
CLAY    2      2650.     .12   1.00E-17  1.00E-17  1.00E-17  2.5   905.5
      1.83e-9  3.47e-5           1.          5.00e-04  5.00E-04
      7          0.4        0.5       1.0       0.05
      7          0.4        0.5       5.6e-7           1.0
CONTA   2      2650.     .17   1.00E-17  1.00E-17  1.00E-17  52.0   905.5
      1.83e-9  3.47e-5           1.          5.00e-04  5.00E-04
...
MULTI---1-----2-----3-----4-----5-----6-----7-----8
?      ?      2      8
START---1-----2-----3-----4-----5-----6-----7-----8
----*---1 MOP: 123456789*123456789*1234 ----*---5-----6-----7-----8
PARAM---1-----2-----3-----4-----5-----6-----7-----8
 3 10 99991 ??      1.0e+3           9.8
      1.E-04  1.E+0
      6.37E6   1.0e-3           0.0           0.0
      0.0      25.0
SELECT---1-----2-----3-----4-----5-----6-----7-----8
 6 1 24 2
  -1.e5
      0.e-0   0.e-1
      0.e-9   0.e-9   1.e-5   0.0e-9   0.e-9   1.e-11
      1.8e11   ??   1.e-5   1.0e-9           ???
      1.0e30   ??   1.e-5   1.0e-9           ???
...
```

Portion of input file for *SimRad2.txt*.

42

21

```

GENER-----1-----2-----3-----4-----5-----6-----7-----8
AL1 LAIR 1   ?    1      ????    ?
AM1 LAIR 1   ?    1      ????    ?
AN1 LAIR 1   ?    1      ????    ?
AO1 LAIR 1   ?    1      ????    ?
AP1 LAIR 1   ?    1      ????    ?
AQ1 LAIR 1   ?    1      ????    ?
AR1 LAIR 1   ?    1      ????    ?
AS1 LAIR 1   ?    1      ????    ?
AT1 LAIR 1   ?    1      ????    ?
AU1 LAIR 1   ?    1      ????    ?

INCON -- INITIAL CONDITIONS FOR HYDROSTATIC PROFILE
A21 1          0.12000086E+00
  0.63773919816909E+07 0.9999999999992E-03 0.00000000000000E+00 0.00000000000000E+00
  0.00000000000000E+00 0.25000000000000E+02
A31 1          0.12000172E+00
  0.6377839640616E+07 0.1000000000002E-02 0.00000000000000E+00 0.00000000000000E+00
  0.00000000000000E+00 0.25000000000000E+02
A41 1          0.12000258E+00
  0.6381759471120E+07 0.9999999999907E-03 0.00000000000000E+00 0.00000000000000E+00
  0.00000000000000E+00 0.25000000000000E+02
A51 1          0.12000344E+00
  0.6385679308422E+07 0.9999999999967E-03 0.00000000000000E+00 0.00000000000000E+00
  0.00000000000000E+00 0.25000000000000E+02
A61 1          0.12000409E+00
...

```

Portion of input file for *SimRad2.txt* (cont.)

43

E.1 Radionuclide properties

- Specify the inverse Henry's constant values and the molecular weights of the radionuclides in the SELEC block.
- Check that the K_d values are in the ROCKS block are correct.

E.2 Generation of air

To specify the total rate for a source of air or any other component (^{14}C or heat) in the waste container, the amount injected in each grid block must be calculated accordingly. Since there are 10×10 grid blocks making up the waste container (though only half are modeled, due to symmetry), the rate for each grid block is calculated by dividing the total rate for the waste container by 100.

44

The first line of the GENER block begins with element “AL1 1”, followed by the source name (“AIR 1”) and the parameter NSEQ (currently “?”). NSEQ is the number of additional sources that will be created by adding a number (NADD) to the element name. For example, to specify additional sources for elements AL1 2, and AL1 3, then NSEQ would be 2 and NADD would be 1.

- Make NSEQ = 4 for each of the lines in the GENER block since there are 4 additional columns of elements that belong to the waste container material (CONTA).
- The parameter TYPE is currently given with “????”. Look in the manual for a description of the different types of sources (or sinks). Pick the right source type to inject air.
- Inject a total of 3.0E-8 kg/s in the waste canister.

45

- Save the file and run the simulator.
- The code should have stopped after MCYC=20 iterations, but print-out should be available in multiples of MCYPR=10 (i.e., after 10 and 20 iterations). Open the main output file (*SimRad2.out*) and scroll down to the first occurrence of “OUTPUT DATA”.

Q-E.2.1: Has the gas phase evolved in any elements by this time? Explain why this is the case.

Q-E.2.2: Scroll down to the next occurrence of “OUTPUT DATA” and verify that the gas phase has formed in the waste canister. Now open the SAVE file and explain how one can tell which elements contain the gas phase.

46

E.3 Generation of ^{14}C and heat in waste container

In this step, the GENER block will be further modified to initiate injection of ^{14}C (total of 1.0E-11 kg/s) and heat (total of 100 W/m).

Q-E.3.1: What option of parameter TYPE is needed for ^{14}C and for heat? (Hint: which primary variable is ^{14}C ?)

- Add two new sets of entries in the GENER block for ^{14}C and heat. Copy the information at the bottom of *SimRad2.txt* file and paste it into the GENER block under the air sources from the previous step. Fill in the remaining information (find the "?").

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E.4 Simulating pressure build-up inside of bentonite seal

- Increase (MCYC=9999) iterations, and make print-out occur at end of simulation (MCYPR=9999).
- Set maximum simulation time (TIMAX in PARAM.2) to 5.0E8 seconds (~15.8 years).
- Use the FOFT block to print time-dependent data to a file (also called FOFT) for two elements, “AO1_1” and “AE1_1”. These elements are located in the first column in the waste container and in the host rock, respectively.
- Save file as *SimRad2_1.txt* and run code. (May take several minutes to run.) Rename the SAVE file as *SAVE_SimRad2_1*.

48

Q-E.4.1: Has the gas migrated through the bentonite seal? What is the pressure inside the waste container and is it likely to cause fracturing in reality? (Hint: fracturing is likely when the pressure exceeds the lithostatic pressure, which is approximately two times the hydrostatic pressure.)

Q-E.4.2: What was the total mass of ^{14}C (Rn1) and ^{14}N (Rn2) at the beginning and end of the simulation?

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E.5 Simulating pressure release following “formation” of fracture through bentonite

While the basic module of TOUGH2 cannot simulate the formation of fractures, let us assume that the increased pressure observed in the previous step was enough to cause a vertical fracture through the bentonite seal.

- Save the file as *SimRad2_2.txt*
- Go to the **ELEME** block and change parameter **MA2**, which specifies the material properties, from bentonite (**BENTO**) to clay (**CLAY**) for the first column only. This thin column of elements will serve as a fracture through the bentonite allowing a connection to the host rock.
- Copy the initial conditions from *SAVE_SimRad2_1* to the **INCON** block. This time keep the continuation information following the “+++”

50

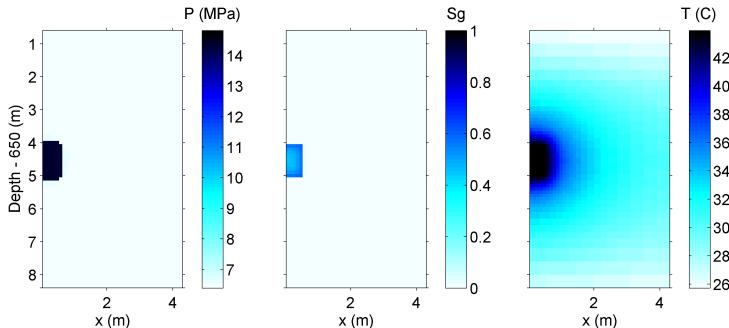
- Set the total simulation time to 5.01728E8 seconds (~15.8 years + 20 days).
- Save file and run the code. (May take several minutes to run.)

Q-E.5.1: Has the pressure decreased inside the waste container?

Q-E.5.2: Has fracture allowed gas to migrate beyond the bentonite seal in this short simulation time?

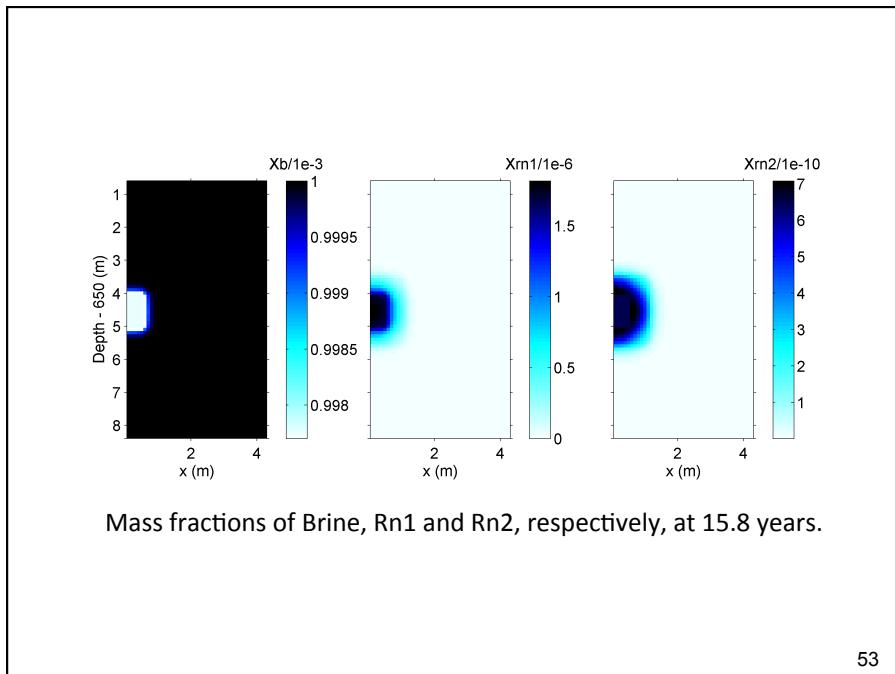
The following figures depict distributions of pressure, gas saturation, temperature, and radionuclide mass fractions from SAVE files for various steps performed above. They also show the pressure and radionuclide transport response (from FOFT files) before and after the “fracture” was incorporated into the flow model.

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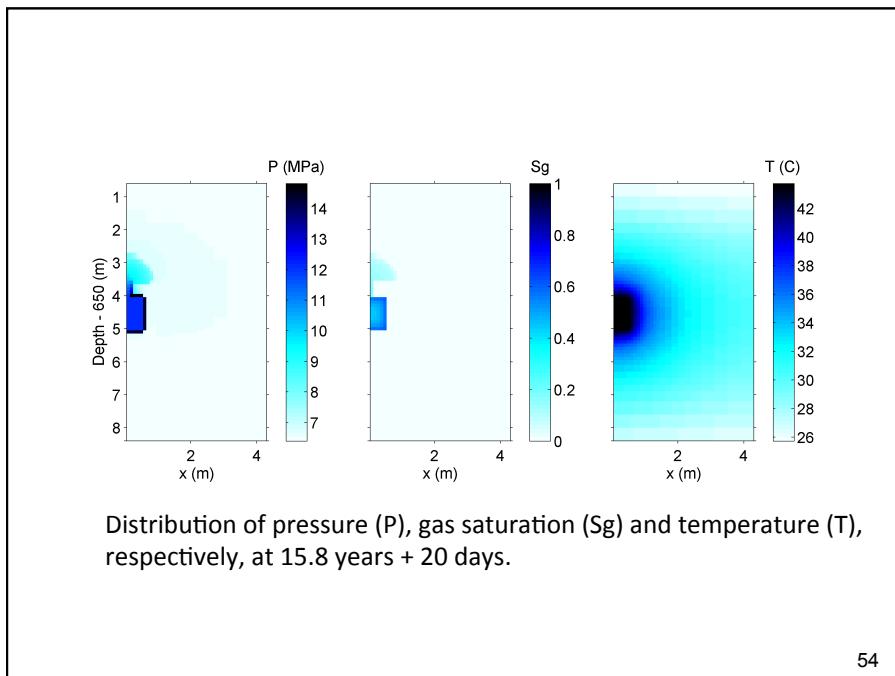


Distribution of pressure (P), gas saturation (Sg) and temperature (T), respectively, at 15.8 years.

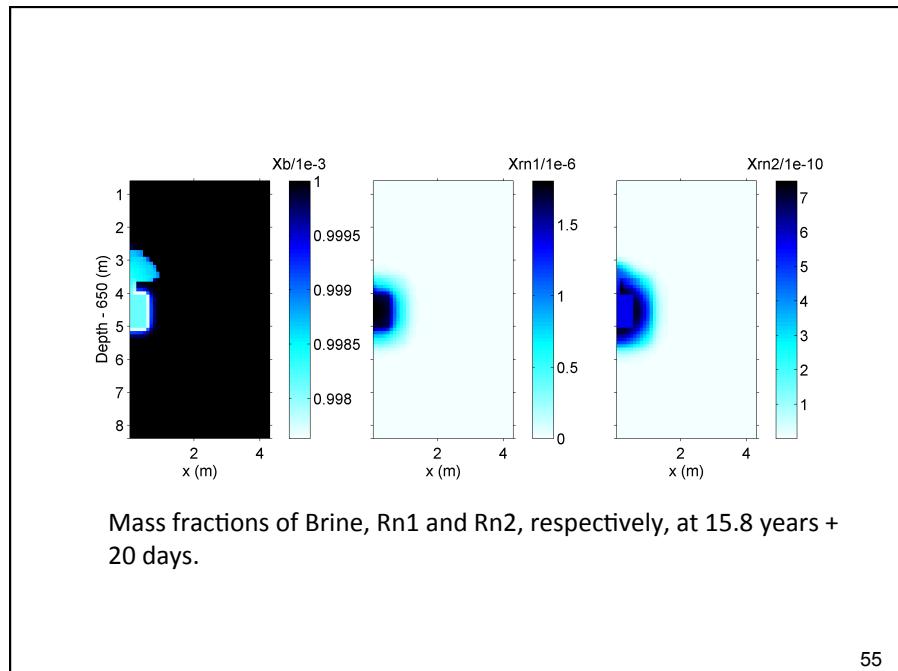
52



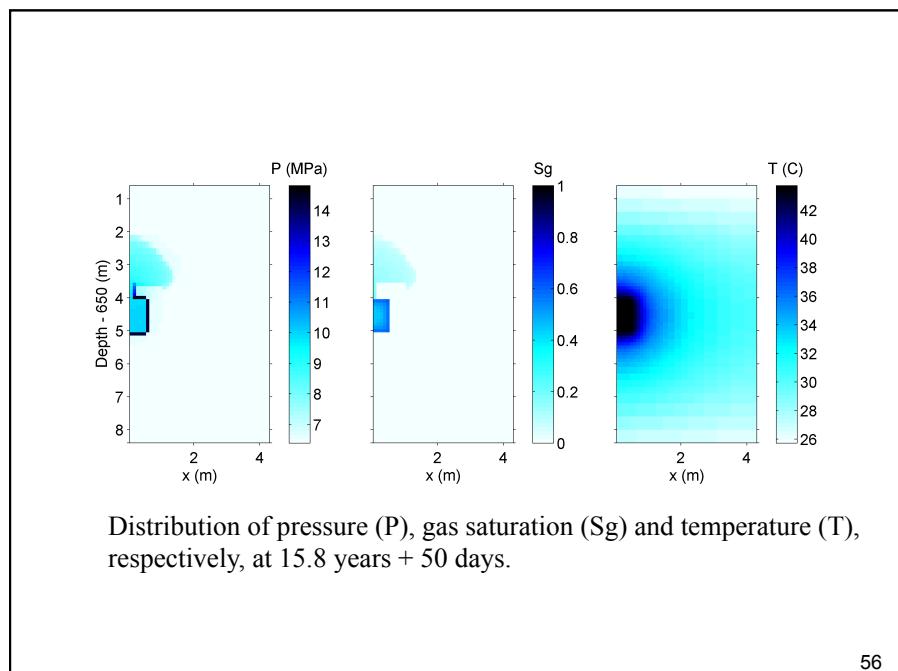
53



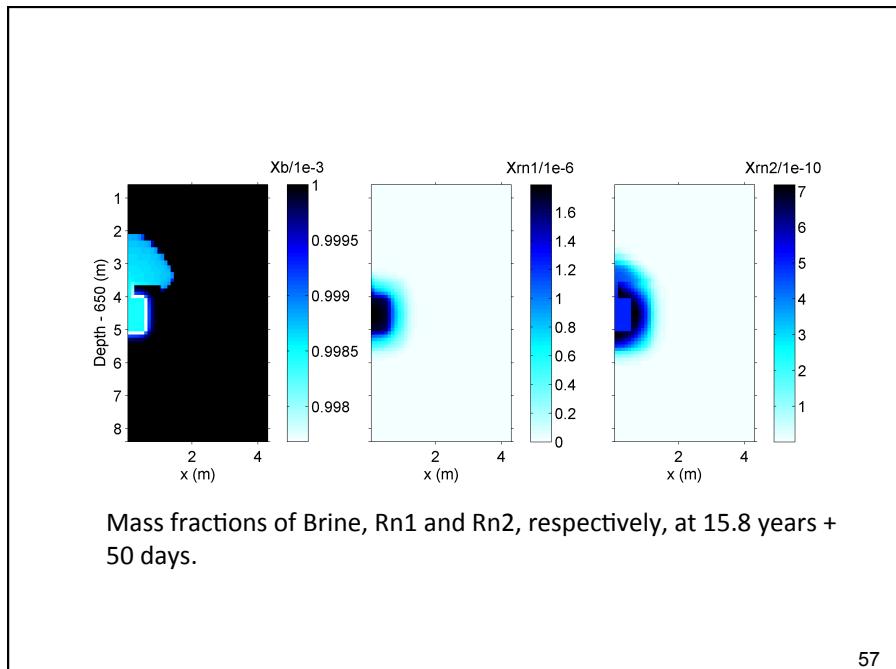
54



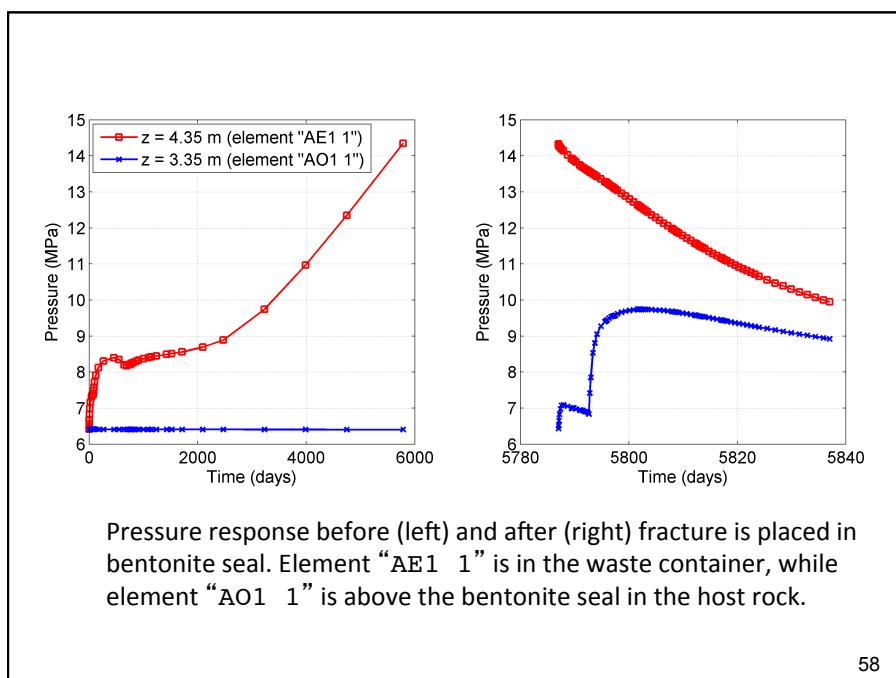
55



56

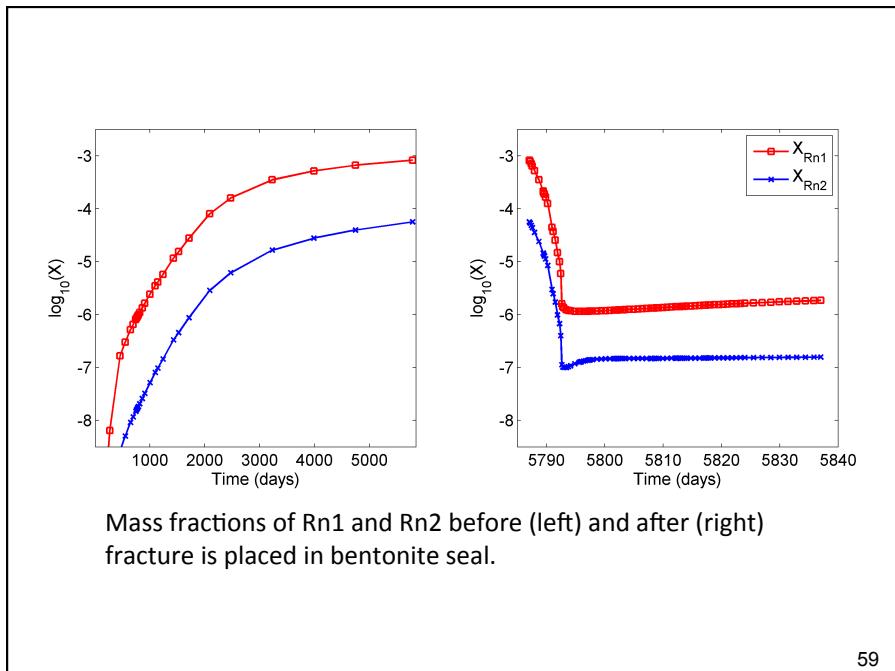


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29



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TOUGH Short Course

Lawrence Berkeley National Laboratory
Earth Sciences Division
Berkeley, California

Selected Input and Output Files for EOS7R Problem

- Files for Part A: *MatDist.txt*
- Files for Part B: *MakeMesh.txt, MESH_1D, MESH_2D, MESH_MatNum*
- Files for Part C: *SimInit.txt, SimInit.out, SAVE_SimInit, SimInit_Flow.txt*
- Files for Part D: *SimRad1_Flow.txt*
- Files for Part E: *SimRad2_1.txt, SimRad2_2.txt, SimRad2_2.out*

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Part A (MatDist.txt)

```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
CLAY    2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5    905.5
       1.83e-9  3.47e-5           1.          1.00e-00  1.00E-03
       7        0.4      0.5      1.0      0.05
       7        0.4      0.5      5.6e-7           1.0
CONTA   2      2650.     .17   1.00E-17  1.00E-17  1.00E-17   52.0   905.5
       1.83e-9  3.47e-5           1.          1.00e-00  1.00E-03
       7        0.4      0.3      1.          0.05
       7        0.4      0.3      1.E-5           1.0
BENTO   2      2650.     .40   1.00E-20  1.00E-20  1.00E-20   1.35   964.0
       3.58e-9  1.5e-5           1.          1.00e-00  1.00E-03
       7        0.4      0.3      1.          0.05
       7        0.4      0.3      5.6e-9           1.0
TOPBC   2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5    905.5
       1.83e-9  3.47e-5           1.          1.00e-00  1.00E-03
       7        0.4      0.5      1.          0.05
       7        0.4      0.5      5.6e-7           1.0
BOTBC   2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5    905.5
       1.83e-9  3.47e-5           1.          1.00e-00  1.00E-03
       7        0.4      0.5      1.          0.05
       7        0.4      0.5      5.6e-7           1.0
MULTI---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
?      ?      2      8
START---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
-----*---1 MOP: 123456789*123456789*1234 -----*---5-----*---6-----*---7-----*---8
PARAM---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
39999  99991      4      5      1.0e-1      9.8
      1.E-05    1.E+0      5.00E6      0.0      0.0      0.0
      25.0
```

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```
SELEC---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
6      1      24      2
      -1.e5

      0.e-0      0.e-1
      0.e-9      0.e-9      1.e-5      0.0e-9      0.e-9      1.e-11
      1.0e1      1.0      0.e-6      1.162e-9           1.e+30
      1.0e1      1.0      0.e-6      1.162e-9           1.e+30

GENER---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
INCON---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
*****
Add ELEM and CONNE blocks here
*****
```

ENDCY

```
*****
When needed, move the INDOM block given below to below GENER block
*****
INDOM---1-----*---2-----*---3-----*---4-----*---5-----*---6-----*---7-----*---8
?????      0.12000086E+00
      0.50000000000000E+07  0.00000000000000E-00  0.00000000000000E+00  0.00000000000000E+00
      0.25000000000000E+02
```

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Part B (MESH_1D)

ELEM		
A11 1	10.1000E+000.2000E+00	0.5000E-010.5000E+00-.5000E+00
A11 2	10.1000E+000.2000E+00	0.1500E+000.5000E+00-.5000E+00
A11 3	10.1000E+000.2000E+00	0.2500E+000.5000E+00-.5000E+00
A11 4	10.1000E+000.2000E+00	0.3500E+000.5000E+00-.5000E+00
A11 5	10.1000E+000.2000E+00	0.4500E+000.5000E+00-.5000E+00
A11 6	10.1000E+000.2000E+00	0.5500E+000.5000E+00-.5000E+00
A11 7	10.1000E+000.2000E+00	0.6500E+000.5000E+00-.5000E+00
A11 8	10.1000E+000.2000E+00	0.7500E+000.5000E+00-.5000E+00
A11 9	10.1000E+000.2000E+00	0.8500E+000.5000E+00-.5000E+00
A1110	10.1000E+000.2000E+00	0.9500E+000.5000E+00-.5000E+00
A1111	10.1000E+000.2000E+00	0.1050E+010.5000E+00-.5000E+00
A1112	10.1000E+000.2000E+00	0.1150E+010.5000E+00-.5000E+00
A1113	10.1000E+000.2000E+00	0.1250E+010.5000E+00-.5000E+00
A1114	10.1000E+000.2000E+00	0.1350E+010.5000E+00-.5000E+00
A1115	10.1000E+000.2000E+00	0.1450E+010.5000E+00-.5000E+00
A1116	10.2000E+000.4000E+00	0.1600E+010.5000E+00-.5000E+00
A1117	10.2000E+000.4000E+00	0.1800E+010.5000E+00-.5000E+00
A1118	10.2000E+000.4000E+00	0.2000E+010.5000E+00-.5000E+00
A1119	10.2000E+000.4000E+00	0.2200E+010.5000E+00-.5000E+00
A1120	10.2000E+000.4000E+00	0.2400E+010.5000E+00-.5000E+00
A1121	10.4000E+000.8000E+00	0.2700E+010.5000E+00-.5000E+00
A1122	10.4000E+000.8000E+00	0.3100E+010.5000E+00-.5000E+00
A1123	10.4000E+000.8000E+00	0.3500E+010.5000E+00-.5000E+00
A1124	10.4000E+000.8000E+00	0.3900E+010.5000E+00-.5000E+00
A1125	10.4000E+000.8000E+00	0.4300E+010.5000E+00-.5000E+00
CONNE		
A11 1A11 2		10.5000E-010.5000E-010.1000E+01
A11 2A11 3		10.5000E-010.5000E-010.1000E+01
A11 3A11 4		10.5000E-010.5000E-010.1000E+01
A11 4A11 5		10.5000E-010.5000E-010.1000E+01
...		

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Part B (MESH_2D)

ELEM		
A11 1	10.4000E-010.1000E+00	0.5000E-010.5000E+00-.2000E+00
A21 1	10.4000E-010.0000E+00	0.5000E-010.5000E+00-.6000E+00
A31 1	10.4000E-010.0000E+00	0.5000E-010.5000E+00-.1000E+01
A41 1	10.4000E-010.0000E+00	0.5000E-010.5000E+00-.1400E+01
A51 1	10.4000E-010.0000E+00	0.5000E-010.5000E+00-.1800E+01
A61 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.2100E+01
A71 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.2300E+01
A81 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.2500E+01
A91 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.2700E+01
AA1 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.2900E+01
AB1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3050E+01
AC1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3150E+01
AD1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3250E+01
AE1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3350E+01
AF1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3450E+01
AG1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3550E+01
AH1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3650E+01
AI1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3750E+01
AJ1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3850E+01
AK1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.3950E+01
AL1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4050E+01
AM1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4150E+01
AN1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4250E+01
AO1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4350E+01
AP1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4450E+01
AQ1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4550E+01
AR1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4650E+01
AS1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4750E+01
AT1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4850E+01
AU1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.4950E+01
AV1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5050E+01
AW1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5150E+01

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AX1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5250E+01
AY1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5350E+01
AZ1 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5450E+01
B11 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5550E+01
B21 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5650E+01
B31 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5750E+01
B41 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5850E+01
B51 1	10.1000E-010.0000E+00	0.5000E-010.5000E+00-.5950E+01
B61 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.6100E+01
B71 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.6300E+01
B81 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.6500E+01
B91 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.6700E+01
BA1 1	10.2000E-010.0000E+00	0.5000E-010.5000E+00-.6900E+01
BB1 1	10.4000E-010.0000E+00	0.5000E-010.5000E+00-.7200E+01
BC1 1	10.4000E-010.0000E+00	0.5000E-010.5000E+00-.7600E+01
BD1 1	10.4000E-010.0000E+00	0.5000E-010.5000E+00-.8000E+01
BE1 1	10.4000E-010.0000E+00	0.5000E-010.5000E+00-.8400E+01
BF1 1	10.4000E-010.1000E+00	0.5000E-010.5000E+00-.8800E+01
A11 2	10.4000E-010.1000E+00	0.1500E+000.5000E+00-.2000E+00
A21 2	10.4000E-010.0000E+00	0.1500E+000.5000E+00-.6000E+00
A31 2	10.4000E-010.0000E+00	0.1500E+000.5000E+00-.1000E+01
A41 2	10.4000E-010.0000E+00	0.1500E+000.5000E+00-.1400E+01
A51 2	10.4000E-010.0000E+00	0.1500E+000.5000E+00-.1800E+01
A61 2	10.2000E-010.0000E+00	0.1500E+000.5000E+00-.2100E+01
A71 2	10.2000E-010.0000E+00	0.1500E+000.5000E+00-.2300E+01
A81 2	10.2000E-010.0000E+00	0.1500E+000.5000E+00-.2500E+01
A91 2	10.2000E-010.0000E+00	0.1500E+000.5000E+00-.2700E+01
AA1 2	10.2000E-010.0000E+00	0.1500E+000.5000E+00-.2900E+01
AB1 2	10.1000E-010.0000E+00	0.1500E+000.5000E+00-.3050E+01
AC1 2	10.1000E-010.0000E+00	0.1500E+000.5000E+00-.3150E+01
AD1 2	10.1000E-010.0000E+00	0.1500E+000.5000E+00-.3250E+01
AE1 2	10.1000E-010.0000E+00	0.1500E+000.5000E+00-.3350E+01
AF1 2	10.1000E-010.0000E+00	0.1500E+000.5000E+00-.3450E+01
AG1 2	10.1000E-010.0000E+00	0.1500E+000.5000E+00-.3550E+01
AH1 2	10.1000E-010.0000E+00	0.1500E+000.5000E+00-.3650E+01
...		

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BB125	10.1600E+000.0000E+00	0.4300E+010.5000E+00-.7200E+01
BC125	10.1600E+000.0000E+00	0.4300E+010.5000E+00-.7600E+01
BD125	10.1600E+000.0000E+00	0.4300E+010.5000E+00-.8000E+01
BE125	10.1600E+000.0000E+00	0.4300E+010.5000E+00-.8400E+01
BF125	10.1600E+000.4000E+00	0.4300E+010.5000E+00-.8800E+01
CONNE		
A11 1A11 2	10.5000E-010.5000E-010.4000E+00	
A11 1A21 1	30.2000E+000.2000E+000.1000E+000.1000E+01	
A21 1A21 2	10.5000E-010.5000E-010.4000E+00	
A21 1A31 1	30.2000E+000.2000E+000.1000E+000.1000E+01	
A31 1A31 2	10.5000E-010.5000E-010.4000E+00	
A31 1A41 1	30.2000E+000.2000E+000.1000E+000.1000E+01	
A41 1A41 2	10.5000E-010.5000E-010.4000E+00	
A41 1A51 1	30.2000E+000.2000E+000.1000E+000.1000E+01	
A51 1A51 2	10.5000E-010.5000E-010.4000E+00	
A51 1A61 1	30.2000E+000.1000E+000.1000E+000.1000E+01	
A61 1A61 2	10.5000E-010.5000E-010.2000E+00	
A61 1A71 1	30.1000E+000.1000E+000.1000E+000.1000E+01	
A71 1A71 2	10.5000E-010.5000E-010.2000E+00	
A71 1A81 1	30.1000E+000.1000E+000.1000E+000.1000E+01	
A81 1A81 2	10.5000E-010.5000E-010.2000E+00	
A81 1A91 1	30.1000E+000.1000E+000.1000E+000.1000E+01	
A91 1A91 2	10.5000E-010.5000E-010.2000E+00	
A91 1AA1 1	30.1000E+000.1000E+000.1000E+000.1000E+01	
AA1 1AA1 2	10.5000E-010.5000E-010.2000E+00	
AA1 1AB1 1	30.1000E+000.5000E-010.1000E+000.1000E+01	
AB1 1AB1 2	10.5000E-010.5000E-010.1000E+00	
AB1 1AC1 1	30.5000E-010.5000E-010.1000E+000.1000E+01	
AC1 1AC1 2	10.5000E-010.5000E-010.1000E+00	
AC1 1AD1 1	30.5000E-010.5000E-010.1000E+000.1000E+01	
AD1 1AD1 2	10.5000E-010.5000E-010.1000E+00	
AD1 1AE1 1	30.5000E-010.5000E-010.1000E+000.1000E+01	
AE1 1AE1 2	10.5000E-010.5000E-010.1000E+00	
...		

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Part C (SimInit.txt)

```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS---1-----2-----3-----4-----5-----6-----7-----8
CLAY    2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5   905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7        0.4        0.5        1.0        0.05
       7        0.4        0.5        5.6e-7          1.0
CONTA   2      2650.     .17   1.00E-17  1.00E-17  1.00E-17   52.0   905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7        0.4        0.3        1.          0.05
       7        0.4        0.3        1.E-5          1.0
BENTO   2      2650.     .40   1.00E-20  1.00E-20  1.00E-20   1.35   964.0
       3.58e-9  1.5e-5          1.          1.00e-00  1.00E-03
       7        0.4        0.3        1.          0.05
       7        0.4        0.3        5.6e-9          1.0
TOPBC   2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5   905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7        0.4        0.5        1.          0.05
       7        0.4        0.5        5.6e-7          1.0
BOTBC   2      2650.     .12   1.00E-17  1.00E-17  1.00E-17   2.5   905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7        0.4        0.5        1.          0.05
       7        0.4        0.5        5.6e-7          1.0
MULTI---1-----2-----3-----4-----5-----6-----7-----8
 4      4      2      8
START---1-----2-----3-----4-----5-----6-----7-----8
-----*---1 MOP: 123456789*123456789*1234 -----*---5-----6-----7-----8
PARAM---1-----2-----3-----4-----5-----6-----7-----8
 39999  99991      4      5      9.8
           1.0e+3
 1.E-05   1.E+0
 6.37E6
 25.0
```

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```
SELEC---1-----2-----3-----4-----5-----6-----7-----8
 6      1      24      2
 -1.e5

 0.e-0    0.e-1
 0.e-9    0.e-9    1.e-5    0.0e-9    0.e-9    1.e-11
 1.0e1    1.0      0.e-6    1.162e-9          1.e+30
 1.0e1    1.0      0.e-6    1.162e-9          1.e+30

GENER---1-----2-----3-----4-----5-----6-----7-----8
INDOM---1-----2-----3-----4-----5-----6-----7-----8
TOPBC   0.12000086E+00
 0.637000000000E+07 1.00000000000000E-03 0.00000000000000E+00 0.00000000000000E+00
 0.250000000000E+02

INCON---1-----2-----3-----4-----5-----6-----7-----8
ELEM
A21 1      10.4000E-010.0000E+00      0.5000E-010.5000E+00-.6000E+00
...
A1123     40.1600E+000.4000E+00      0.3500E+010.5000E+00-.2000E+00
A1124     40.1600E+000.4000E+00      0.3900E+010.5000E+00-.2000E+00
A1125     40.1600E+000.4000E+00      0.4300E+010.5000E+00-.2000E+00
ina
BF1 1      50.4000E-010.1000E+00      0.5000E-010.5000E+00-.8800E+01
BF1 2      50.4000E-010.1000E+00      0.1500E+000.5000E+00-.8800E+01
BF1 3      50.4000E-010.1000E+00      0.2500E+000.5000E+00-.8800E+01
...
BF124     50.1600E+000.4000E+00      0.3900E+010.5000E+00-.8800E+01
BF125     50.1600E+000.4000E+00      0.4300E+010.5000E+00-.8800E+01

CONN
A11 1A11 2      10.5000E-010.5000E-010.4000E+00
A11 1A21 1      30.2000E+000.2000E+000.1000E+000.1000E+01
...
```

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PART C (SAVE_SimInit)

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*****
***** EOSTR: EQUATION OF STATE FOR MIXTURES OF WATER/BRINE/RADIONUCLIDE(1) /RADIONUCLIDE (2) /AIR ****
*****
OPTIONS SELECTED ARE: (NK,NEQ,NPH,NB,NKIN) = (4,4,2,8,4)

      NK = 4 - NUMBER OF COMPONENTS
      NEQ = 4 - NUMBER OF EQUATIONS PER GRID BLOCK
      NPH = 2 - NUMBER OF PHASES THAT CAN BE PRESENT
      NB = 8 - NUMBER OF SECONDARY PARAMETERS (OTHER THAN' COMPONENT MASS FRACTIONS)
      NKIN = 4 - number of components for initializing thermodynamic conditions (default is NKIN = NK)

      For NB = 6, diffusion is "off", for NB = 8, diffusion is "on"

AVAILABLE OPTIONS FOR (NK,NEQ,NPH,NB):
(5,5,2,6 or 8) - WATER, BRINE, RNL, RN2, AIR, ISOTHERMAL;           VARIABLES (P, XB, XRN1, XRN2, X OR S+10, T)
(5,6,2,6 or 8) - WATER, BRINE, RNL, RN2, AIR, NON-ISOTHERMAL;        VARIABLES (P, XB, XRN1, XRN2, X OR S+10, T)
(4,4,2,6 or 8) - WATER, BRINE, RNL, RN2, NO AIR, ISOTHERMAL;        VARIABLES (P, XB, XRN1, XRN2, T)
(4,5,2,6 or 8) - WATER, BRINE, RNL, RN2, NO AIR, NON-ISOTHERMAL;     VARIABLES (P, XB, XRN1, XRN2, T)

NKIN = NK or NKIN = NK-2. Default options are (5,5,2,8) - isothermal, diffusion "on", NKIN=NK

THE NK = 4 ("NO AIR") OPTIONS MAY ONLY BE USED FOR PROBLEMS WITH SINGLE-PHASE LIQUID CONDITIONS THROUGHOUT.

THE NORMAL NUMBER OF SECONDARY PARAMETERS OTHER THAN MASS FRACTIONS IS 6 PER PHASE. IN EOSTR, WE OPTIALLY ADD TO THIS A SATURATION-DEPENDENT TORTUOSITY FOR EACH PHASE, AS WELL AS TEMPERATURE AND PRESSURE DEPENDENCE OF THE DIFFUSION COEFFICIENT.
*****
      NKIN = 4 *** ALLOWS INITIALIZATION WITH DIFFERENT SETS OF PRIMARY VARIABLES. ***
      *** THIS IS USEFUL FOR STARTING EOSTR SIMULATIONS FROM EOSTR INITIAL CONDITIONS. ***
      = NK (default): (P,XB,XRN1,XRN2,XAIR,T) FOR SINGLE PHASE, (P,XB,XRN1,XRN2,S+10,T) FOR TWO-PHASE. (EOSTR FORMAT).
      = NK-2: (P,XB,XAIR,T) FOR SINGLE PHASE, (P,XB,S+10,T) FOR TWO-PHASE. (EOSTR FORMAT). WILL INITIALIZE XRN1 = XRN2 = 0.

*****
THE PRIMARY VARIABLES ARE
P - PRESSURE   T - TEMPERATURE   XB - BRINE MASS FRACTION IN LIQUID (FOR SINGLE-PHASE GAS, XB IS BRINE MASS FRACTION IN GAS)
XRN1 - MASS FRACTION IN THE LIQUID OF RADIONUCLIDE(1) (PARENT)   XRN2 - MASS FRACTION IN THE LIQUID OF RADIONUCLIDE(2) (DAUGHTER)
S+10. - (GAS PHASE SATURATION + 10.)   X - AIR MASS FRACTION   T - TEMPERATURE
*****
      *      COMPONENTS      *
      *      *****      *
      *      # 1 - WATER      *
      *      *      *
      *      # 2 - BRINE       *
      *      *      *
      *      # 3 - RNL         *
      *      *      *
      *      *      FLUID PHASE CONDITION      PRIMARY VARIABLES      *
      *      *****      *
      *      *      *
      *      *      SINGLE-PHASE GAS (#)      P, XB, XRN1, XRN2, X, T      *
      *      *      *
      *      *      SINGLE-PHASE LIQUID (*)      P, XB, XRN1, XRN2, X, T      *
      *      *      *
      *      *      TWO-PHASE (*)      P, XB, XRN1, XRN2, S+10., T      *
      *      *      *

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* # 4 - RN2 *
* # 5 - AIR *
* # 6 - HEAT *
*****
NEGATIVE REFERENCE PRESSURE OF -1.00000E+06 PA WAS SPECIFIED, THUS BRINE PROPERTIES ARE IDENTICAL TO WATER FOR ALL SALINITIES.

PROPERTIES OF THE RADIONUCLIDES: DOMAIN RADIONUCLIDE(1) RADIONUCLIDE(2)
HALF-LIFE (SECONDS): -ALL- 0.1000E+02 0.1000E+02
MOLECULAR WEIGHT (GM/MOLE): -ALL- 0.1000E+01 0.1000E+01
INVERSE HENRY CONST. (MOLE/PA): -ALL- 0.1000E+31 0.1000E+31
GAS PHASE DIFFUSIVITY (M**2/S): -ALL- 0.0000E+00 0.0000E+00
AQ. PHASE DIFFUSIVITY (M**2/S): -ALL- 0.1162E-08 0.1162E-08
DISTRIBUTION COEF. (M**3/KG): CLAY 0.1000E+01 0.1000E+02
DISTRIBUTION COEF. (M**3/KG): CORNA 0.1000E+01 0.1000E+02
DISTRIBUTION COEF. (M**3/KG): BENTO 0.1000E+01 0.1000E+02
DISTRIBUTION COEF. (M**3/KG): TOPBC 0.1000E+01 0.1000E+02
DISTRIBUTION COEF. (M**3/KG): BOTBC 0.1000E+01 0.1000E+02

MOLECULAR DIFFUSIVITY OF WATER, BRINE, XRN1, XRN2, AND AIR THROUGH THE GASEOUS AND AQUEOUS PHASES, (FDIAG(PHASE,COMP)) [M**2/S]: PHASE 1 = GAS; PHASE 2 = AQUEOUS
  PHASE COMP  PHASE COMP
  -1-  -2-  -3-  -4-  -5-  -6-  -7-  -8-  -9-  -10-  -11-  -12-  -13-  -14-  -15-  -16-
  0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1000E-04 0.0000E+00 0.0000E+00 0.1162E-08 0.1162E-08 0.1162E-08 0.1000E-10

***** VOLUME- AND MASS-BALANCES *****
***** [KCYC,ITER] = [ 0, 0 ] ***** THE TIME IS 0.00000E+00 SECONDS, OR 0.00000E+00 DAYS

***** PHASES PRESENT *****
***** PHASES * GAS AQUEOUS PHASES * GAS AQUEOUS COMPONENT MASS IN PLACE (KG) *****
***** PHASES * GAS AQUEOUS ADSORBED TOTAL *****
***** ELEMENTS *****
VOLUME (M**3) * 0.00000000E+00 0.50890000E+01 WATER * 0.00000000E+00 0.50836691E+04 0.00000000E+00 0.50836691E+04
MASS (KG) * 0.00000000E+00 0.50887579E+04 BRINE * 0.00000000E+00 0.50887579E+01 0.00000000E+00 0.50887579E+01
***** RN1 * 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
RN2 * 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
AIR * 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
*****
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B11 1( 1, 1) ST = 0.100000E+04 DX1 = 0.100000E+00 DX2= 0.000000E+00 T = 25.000 P = 6370000 S = 0.000000E+00
...ITERATING.. AT [ 2, 1] --- DELTEX = 0.200000E+04 MAX. RES. = 0.183322E-04 AT ELEMENT B11 1 EQUATION 1
ALL 5( 2, 2) ST = 0.300000E+04 DT = 0.200000E+04 DX1= -1.23165E+04 DX2= 0.453532E-15 T = 25.000 P = 6368768 S = 0.000000E+00
...ITERATING.. AT [ 3, 1] --- DELTEX = 0.400000E+04 MAX. RES. = 0.191969E-04 AT ELEMENT ALL 5 EQUATION 1
ARI 5( 3, 2) ST = 0.700000E+04 DT = 0.400000E+04 DX1= -696863E+02 DX2= 0.861142E-17 T = 25.000 P = 6369362 S = 0.000000E+00
...ITERATING.. AT [ 4, 1] --- DELTEX = 0.500000E+04 MAX. RES. = 0.115820E-04 AT ELEMENT ARI 5 EQUATION 1
BFI( 4, 2) ST = 0.150000E+05 DT = 0.800000E+04 DX1= 0.0007768E+04 DX2= -1.47778E-14 T = 25.000 P = 6376199. S = 0.000000E+00
...ITERATING.. AT [ 5, 1] --- DELTEX = 0.160000E+05 MAX. RES. = 0.160000E+00 AT ELEMENT AG1 1 EQUATION 1
A0111( 5, 2) ST = 0.310000E+05 DT = 0.160000E+05 DX1= 0.716526E+02 DX2= -4.22539E-17 T = 25.000 P = 6370407. S = 0.000000E+00
...ITERATING.. AT [ 6, 1] --- DELTEX = 0.320000E+05 MAX. RES. = 0.193227E-04 AT ELEMENT AG1 1 EQUATION 1
...ITERATING.. AT [ 6, 2] --- DELTEX = 0.320000E+05 MAX. RES. = 0.126633E-03 AT ELEMENT A0111 EQUATION 1

...
ATI 5( 14, 2) ST = 0.163830E+07 DT = 0.819290E+07 DX1= 0.116491E+05 DX2= -202528E-13 T = 25.000 P = 6374478. S = 0.000000E+00
...ITERATING.. AT [ 15, 1] --- DELTEX = 0.1563840E+08 MAX. RES. = 0.974024E-04 AT ELEMENT AV1 6 EQUATION 1
AMM 3( 15, 2) ST = 0.327670E+07 DT = 0.163840E+08 DX1= 0.114330E+05 DX2= 0.449596E-13 T = 25.000 P = 6399323. S = 0.000000E+00
...ITERATING.. AT [ 16, 1] --- DELTEX = 0.327680E+08 MAX. RES. = 0.906828E-04 AT ELEMENT AV1 1 EQUATION 1
ASI 4( 16, 2) ST = 0.655350E+07 DT = 0.327680E+08 DX1= 0.670244E+04 DX2= 0.822832E-15 T = 25.000 P = 6411904. S = 0.000000E+00
...ITERATING.. AT [ 17, 1] --- DELTEX = 0.655360E+08 MAX. RES. = 0.523781E-04 AT ELEMENT AV1 1 EQUATION 1
AQI 5( 17, 2) ST = 0.131071E+09 DT = 0.655360E+08 DX1= 0.228686E+04 DX2= 0.639986E-15 T = 25.000 P = 6412453. S = 0.000000E+00
...ITERATING.. AT [ 18, 1] --- DELTEX = 0.131072E+09 DT = 0.115272E+09 DX1= 0.405378E+03 DX2= 0.123261E-14 T = 25.000 P = 6412454. S = 0.000000E+00
ASI 4( 18, 2) ST = 0.262144E+09 DT = 0.121072E+09 DX1= 0.405378E+03 DX2= 0.123261E-14 T = 25.000 P = 6414548. S = 0.000000E+00
AV1 1( 19, 1) ST = 0.524287E+09 DT = 0.262144E+09 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6417449. S = 0.000000E+00
AV1 1( 20, 1) ST = 0.104485E+10 DT = 0.524287E+09 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6417449. S = 0.000000E+00
...ITERATING.. AT [ 21, 1] --- DELTEX = 0.104485E+10 MAX. RES. = 0.125835E-04 AT ELEMENT AV1 1 EQUATION 1
AMI 4( 21, 2) ST = 0.209715E+10 DT = 0.104485E+10 DX1= 0.390685E+02 DX2= -4.21210E-16 T = 25.000 P = 6408708. S = 0.000000E+00
AV1 1( 22, 1) ST = 0.419430E+10 DT = 0.209715E+10 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6417528. S = 0.000000E+00
AV1 1( 23, 1) ST = 0.838860E+10 DT = 0.419430E+10 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6417528. S = 0.000000E+00
AV1 1( 24, 1) ST = 0.167772E+11 DT = 0.838860E+10 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6417528. S = 0.000000E+00
AV1 1( 25, 1) ST = 0.335544E+11 DT = 0.167772E+11 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6417528. S = 0.000000E+00
AV1 1( 26, 1) ST = 0.671089E+11 DT = 0.335544E+11 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6417528. S = 0.000000E+00
AV1 1( 27, 1) ST = 0.134218E+12 DT = 0.671089E+11 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6417528. S = 0.000000E+00
...ITERATING.. AT [ 28, 1] --- DELTEX = 0.134218E+12 MAX. RES. = 0.197603E-04 AT ELEMENT AV1 1 EQUATION 1
ASI 2( 28, 2) ST = 0.268435E+12 DT = 0.134218E+12 DX1= 0.494625E+00 DX2= 0.944114E-18 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 29, 1) ST = 0.536871E+12 DT = 0.268435E+12 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 30, 1) ST = 0.107374E+13 DT = 0.536871E+12 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 31, 1) ST = 0.214744E+13 DT = 0.107374E+13 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 32, 1) ST = 0.429497E+13 DT = 0.214744E+13 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 33, 1) ST = 0.859939E+13 DT = 0.429497E+13 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 34, 1) ST = 0.171799E+14 DT = 0.859939E+13 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 35, 1) ST = 0.343597E+14 DT = 0.171799E+14 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 36, 1) ST = 0.687195E+14 DT = 0.343597E+14 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
ASI 2( 37, 1) ST = 0.137439E+15 DT = 0.687195E+14 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00
***** FOR 10 CONSECUTIVE TIME STEPS HAVE CONVERGED ON ITER = 1
WRITE OUT CURRENT DATA, THEN STOP EXECUTION
ASI 2( 38, 1) ST = 0.274788E+15 DT = 0.137439E+15 DX1= 0.000000E+00 DX2= 0.000000E+00 T = 25.000 P = 6414588. S = 0.000000E+00

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RADIONUCLIDE TRANSPORT PROBLEM

OUTPUT DATA AFTER (38, 1) -2-TIME STEPS

THE TIME IS 0.318146E+10 DAYS

TOTAL TIME	KCYC	ITER	ITERC	KON	DX1M	DX2M	DX3M	MAX. RES.	NER	KER	DELTEX
0.274878E+15	38	1	62	2	0.00000E+00	0.00000E+00	0.00000E+00	0.94287E-05	75	1	0.13744E+15

ELEM.	INDEX	P (PA)	T (DEG-C)	SL	XBRINE(LIQ)	XRN1(LIQ)	XRN2(LIQ)	XAIRG	XRN1(GAS)	XRN2(GAS)	DL (KG/M**3)
A21	1	0	0.63739E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A31	1	0	0.63778E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A41	3	0	0.43818E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A51	4	0	0.43818E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A61	5	0	0.43818E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A71	6	0	0.63906E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A81	7	0	0.63925E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A91	8	0	0.63945E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A11	9	0	0.63965E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A13	10	0	0.63985E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99996E+03
A15	11	0	0.63998E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
A01	12	0	0.63998E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
A01	13	0	0.64009E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
A01	14	0	0.64018E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AG1	15	0	0.64028E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AH1	16	0	0.64038E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
A11	17	0	0.64048E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AJ1	18	0	0.64058E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AK1	19	0	0.64067E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AL1	20	0	0.64077E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AM1	21	0	0.64087E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AN1	22	0	0.64097E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AP1	23	0	0.64107E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AP1	24	0	0.64116E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AQ1	25	0	0.64126E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AR1	26	0	0.64136E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AS1	27	0	0.64146E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AT1	28	0	0.64156E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AV1	29	0	0.64165E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AV1	30	0	0.64175E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AW1	31	0	0.64185E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AX1	32	0	0.64195E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AY1	33	0	0.64205E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
AZ1	34	0	0.64214E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
B11	35	0	0.64224E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03
B21	36	0	0.64234E+07	0.25000E+02	0.10000E+01	0.10000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.99997E+03

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Part C (SAVE_SimInit)

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INCON -- INITIAL CONDITIONS FOR 1251 ELEMENTS AT TIME 0.274878E+15
A21 1      0.12000086E+00
 0.63739198169098E+07 0.9999999999992E-03 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A31 1      0.12000172E+00
 0.63778396406168E+07 0.1000000000002E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A41 1      0.12000258E+00
 0.6381759471120E+07 0.9999999999907E-03 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A51 1      0.12000344E+00
 0.6385679308422E+07 0.9999999999967E-03 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A61 1      0.12000409E+00
 0.6388619190859E+07 0.9999999999961E-03 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A71 1      0.12000452E+00
 0.6390579114608E+07 0.100000000003E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A81 1      0.12000495E+00
 0.6392539040057E+07 0.9999999999972E-03 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A91 1      0.12000538E+00
 0.6394498967204E+07 0.100000000008E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
...
BE1 1      0.12001765E+00
 0.6450357605269E+07 0.1000000000038E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A21 2      0.12000086E+00
 0.63739198169098E+07 0.1000000000001E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
...

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...
BF122      0.12001851E+00
 0.6454277561522E+07 0.1000000000005E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
BF123      0.12001851E+00
 0.6454277561522E+07 0.1000000000042E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
BF124      0.12001851E+00
 0.6454277561522E+07 0.9999999999972E-03 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
BF125      0.12001851E+00
 0.6454277561522E+07 0.1000000000024E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
ina 0      0.12000000E+00
 0.6370000000000E+07 0.1000000000000E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A11 1      0.12000000E+00
 0.6370000000000E+07 0.1000000000000E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A11 2      0.12000000E+00
 0.6370000000000E+07 0.1000000000000E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
...
A1123     0.12000000E+00
 0.6370000000000E+07 0.1000000000000E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A1124     0.12000000E+00
 0.6370000000000E+07 0.1000000000000E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
A1125     0.12000000E+00
 0.6370000000000E+07 0.1000000000000E-02 0.0000000000000E+00 0.0000000000000E+00
 0.2500000000000E+02
+++
 38      62      5 0.00000000E+00 0.27487791E+15

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Part C (SimInit_Flow.txt)

```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8
CLAY    2      2650.     .12   1.00E-17  1.00E-17  1.00E-17  2.5     905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7          0.4          0.5          1.0          0.05
       7          0.4          0.5          5.6e-7          1.0
CONTA   2      2650.     .17   1.00E-17  1.00E-17  1.00E-17  52.0    905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7          0.4          0.3          1.          0.05
       7          0.4          0.3          1.E-5          1.0
BENTO   2      2650.     .40   1.00E-20  1.00E-20  1.00E-20  1.35    964.0
       3.58e-9  1.5e-5          1.          1.00e-00  1.00E-03
       7          0.4          0.3          1.          0.05
       7          0.4          0.3          5.6e-9          1.0
TOPEC   2      2650.     .12   1.00E-17  1.00E-17  1.00E-17  2.5     905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7          0.4          0.5          1.          0.05
       7          0.4          0.5          5.6e-7          1.0
BOTBC   2      2650.     .12   1.00E-17  1.00E-17  1.00E-17  2.5     905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7          0.4          0.5          1.          0.05
       7          0.4          0.5          5.6e-7          1.0

MULTI---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8
        4      4      2      8
START---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8
-----*---1 MOP: 123456789*123456789*1234 -----*---5----*---6----*---7----*---8
PARAM---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8
      39999   99991      4      5           1.0e+3           9.8
      1.E-05   1.E+0           6.37E6           0.0           0.0           0.0
      25.0
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SELEC---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8
      6      1      24      2
      -1.e5

      0.e-0      0.e-1
      0.e-9      0.e-9      1.e-5      0.0e-9      0.e-9      1.e-11
      1.0e1      1.0          0.e-6      1.162e-9          1.e+30
      1.0e1      1.0          0.e-6      1.162e-9          1.e+30

GENER---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8

INDOM---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8
TOPBC      0.12000086E+00
      0.637000000000E+07  1.00000000000000E-03  0.00000000000000E+00  0.00000000000000E+00
      0.250000000000E+02
BOTBC      0.12000086E+00
      0.630000000000E+07  1.00000000000000E-03  0.00000000000000E+00  0.00000000000000E+00
      0.250000000000E+02

INCON---1----*---2----*---3----*---4----*---5----*---6----*---7----*---8

ELEME
A21 1      10.4000E-010.0000E+00      0.5000E-010.5000E+00-.6000E+00
...
ina
BF1 1      50.4000E-010.1000E+00      0.5000E-010.5000E+00-.8800E+01
BF1 2      50.4000E-010.1000E+00      0.1500E+000.5000E+00-.8800E+01
BF1 3      50.4000E-010.1000E+00      0.2500E+000.5000E+00-.8800E+01
BF1 4      50.4000E-010.1000E+00      0.3500E+000.5000E+00-.8800E+01
BF1 5      50.4000E-010.1000E+00      0.4500E+000.5000E+00-.8800E+01
BF1 6      50.4000E-010.1000E+00      0.5500E+000.5000E+00-.8800E+01
BF1 7      50.4000E-010.1000E+00      0.6500E+000.5000E+00-.8800E+01
...
```

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Part D (SimRad1_Flow.txt)

```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS---1-----2-----3-----4-----5-----6-----7-----8
CLAY    2      2650.     .12   1.00E-17  1.00E-17  1.00E-17  2.5   905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7         0.4        0.5        1.0        0.05
       7         0.4        0.5        5.6e-7          1.0
CONTA   2      2650.     .17   1.00E-17  1.00E-17  1.00E-17  52.0   905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7         0.4        0.3        1.          0.05
       7         0.4        0.3        1.E-5          1.0
BENTO   2      2650.     .40   1.00E-20  1.00E-20  1.00E-20  1.35   964.0
       3.58e-9  1.5e-5          1.          1.00e-00  1.00E-03
       7         0.4        0.3        1.          0.05
       7         0.4        0.3        5.6e-9          1.0
TOPBC   2      2650.     .12   1.00E-17  1.00E-17  1.00E-17  2.5   905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7         0.4        0.5        1.          0.05
       7         0.4        0.5        5.6e-7          1.0
BOTBC   2      2650.     .12   1.00E-17  1.00E-17  1.00E-17  2.5   905.5
       1.83e-9  3.47e-5          1.          1.00e-00  1.00E-03
       7         0.4        0.5        1.          0.05
       7         0.4        0.5        5.6e-7          1.0
MULTI---1-----2-----3-----4-----5-----6-----7-----8
 4      4      2      8
START---1-----2-----3-----4-----5-----6-----7-----8
-----*---1 MOP: 123456789*123456789*1234 -----*---5-----6-----7-----8
PARAM---1-----2-----3-----4-----5-----6-----7-----8
 39999  99991           4      5           9.8
       6.3072e+10  1.0e+1
       1.E-05    1.E+0
       6.37E6    1.0e-3
       25.0

```

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```
SELEC---1-----2-----3-----4-----5-----6-----7-----8
 6      1      24     2
       -1.e5

       0.e-0    0.e-1
       0.e-9    0.e-9    1.e-5    0.0e-9    0.e-9    1.e-11
 1.44e+10  241.0   0.e-6   1.162e-9          1.e+30
 6.0e+13   237.0   0.e-6   1.162e-9          1.e+30

GENER---1-----2-----3-----4-----5-----6-----7-----8

INCON -- INITIAL CONDITIONS FOR 1251 ELEMENTS AT TIME  0.687195E+15
A21 1          0.11999874E+00
 0.6364272842591E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
A31 1          0.11999751E+00
 0.63586439592288E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
A41 1          0.11999632E+00
 0.6353230232886E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
A51 1          0.11999521E+00
 0.6348192292583E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
A61 1          0.11999448E+00
 0.6344880065463E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
A71 1          0.11999405E+00
 0.6342903223578E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
A81 1          0.11999368E+00
 0.6341224084628E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
...

```

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```

AH1 1      0.39994129E+00
0.6329000804083E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
A11 1      0.39992342E+00
0.6316519125714E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
AJ1 1      0.39990558E+00
0.6304054632497E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
AK1 1      0.39988766E+00
0.6291539927000E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
AL1 1      0.16997168E+00
0.6278967637406E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
AM1 1      0.16997198E+00
0.6279932630210E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
AN1 1      0.16997228E+00
0.6280896469789E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
AO1 1      0.16997258E+00
0.6281859446290E+07 0.100000000000E-02 1.000000000000E-03 0.000000000000E+00
0.250000000000E+02
AP1 1      0.16997288E+00
0.6282821872975E+07 0.100000000000E-02 1.000000000000E-03 0.000000000000E+00
0.250000000000E+02
AQ1 1      0.16997318E+00
0.6283784072965E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
AR1 1      0.16997348E+00
0.6284746392687E+07 0.100000000000E-02 0.000000000000E+00 0.000000000000E+00
0.250000000000E+02
...

```

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Part E (SimRad2_1.txt)

```

*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
CLAY     2      2650.    .12   1.00E-17  1.00E-17  1.00E-17    2.5    905.5
1.83e-9  3.47e-5          1.          5.00e-04  5.00E-04
7         0.4       0.5       1.0       0.05
7         0.4       0.5       5.6e-7          1.0
CONTA    2      2650.    .17   1.00E-17  1.00E-17  1.00E-17    52.0   905.5
1.83e-9  3.47e-5          1.          5.00e-04  5.00E-04
7         0.4       0.3       1.          0.05
7         0.4       0.3       1.E-5          1.0
BENTO    2      2650.    .40   1.00E-20  1.00E-20  1.00E-20    1.35   964.0
3.58e-9  1.5e-5          1.          5.00e-04  5.00E-04
7         0.4       0.3       1.          0.05
7         0.4       0.3       5.6e-9          1.0
TOPBC   2      2650.    .12   1.00E-17  1.00E-17  1.00E-17    2.5    905.5
1.83e-9  3.47e-5          1.          5.00e-04  5.00E-04
7         0.4       0.5       1.          0.05
7         0.4       0.5       5.6e-7          1.0
BOTBC   2      2650.    .12   1.00E-17  1.00E-17  1.00E-17    2.5    905.5
1.83e-9  3.47e-5          1.          5.00e-04  5.00E-04
7         0.4       0.5       1.          0.05
7         0.4       0.5       5.6e-7          1.0

MULTI---1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
5       6       2       8
START---1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
-----1 MOP: 123456789*123456789*1234 -----5-----6-----7-----8
PARAM---1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
39999   99991           4      5
5.0e+8    1.0e+3          9.8
1.E-04    1.E+0            0.0
6.37E6    1.0e-3          0.0
0.0        25.0

```

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```

SELEC----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
   6      1     24      2
   -1.e5

   0.e-0      0.e-1
   0.e-9      0.e-9      1.e-5      0.0e-9      0.e-9      1.e-11
   1.8e11     14.0       1.e-5      1.0e-9
   1.0e30     14.0       1.e-5      1.0e-9
FOFT ----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
AE1 1
AO1 1

GENER----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
ALL 1AIR 1    4      1           COM5      3.0e-10
AM1 1AIR 1    4      1           COM5      3.0e-10
AN1 1AIR 1    4      1           COM5      3.0e-10
AO1 1AIR 1    4      1           COM5      3.0e-10
AP1 1AIR 1    4      1           COM5      3.0e-10
AQ1 1AIR 1    4      1           COM5      3.0e-10
AR1 1AIR 1    4      1           COM5      3.0e-10
AS1 1AIR 1    4      1           COM5      3.0e-10
AT1 1AIR 1    4      1           COM5      3.0e-10
AU1 1AIR 1    4      1           COM5      3.0e-10
ALL 1C14 1    4      1           COM3      1.0e-13
AM1 1C14 1    4      1           COM3      1.0e-13
AN1 1C14 1    4      1           COM3      1.0e-13
AO1 1C14 1    4      1           COM3      1.0e-13
AP1 1C14 1    4      1           COM3      1.0e-13
AQ1 1C14 1    4      1           COM3      1.0e-13
AR1 1C14 1    4      1           COM3      1.0e-13
AS1 1C14 1    4      1           COM3      1.0e-13
AT1 1C14 1    4      1           COM3      1.0e-13
AU1 1C14 1    4      1           COM3      1.0e-13
ALL 1HEA 1    4      1           HEAT      1.00
AM1 1HEA 1    4      1           HEAT      1.00
...

```

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```

AO1 1HEA 1    4      1           HEAT      1.00
AP1 1HEA 1    4      1           HEAT      1.00
AQ1 1HEA 1    4      1           HEAT      1.00
AR1 1HEA 1    4      1           HEAT      1.00
AS1 1HEA 1    4      1           HEAT      1.00
AT1 1HEA 1    4      1           HEAT      1.00
AU1 1HEA 1    4      1           HEAT      1.00

INCON -- INITIAL CONDITIONS FOR 1251 ELEMENTS AT TIME  0.274878E+15
A21 1          0.12000086E+00
  0.6373919816909E+07  0.9999999999992E-03  0.000000000000E+00  0.000000000000E+00
  0.000000000000E+00  0.250000000000E+02
A31 1          0.12000172E+00
  0.6377839640616E+07  0.1000000000002E-02  0.000000000000E+00  0.000000000000E+00
  0.000000000000E+00  0.250000000000E+02
A41 1          0.12000258E+00
  0.6381759471120E+07  0.9999999999907E-03  0.000000000000E+00  0.000000000000E+00
  0.000000000000E+00  0.250000000000E+02
A51 1          0.12000344E+00
  0.6385679308422E+07  0.9999999999967E-03  0.000000000000E+00  0.000000000000E+00
  0.000000000000E+00  0.250000000000E+02
A61 1          0.12000409E+00
...

```

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Part E (SimRad2_2.txt)

```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS---1----2----3----4----5----6----7----8
CLAY    2     2650.   .12  1.00E-17  1.00E-17  1.00E-17   2.5   905.5
      1.83e-9  3.47e-5           1.          5.00e-04  5.00E-04
      7       0.4       0.5       1.0       0.05
      7       0.4       0.5       5.6e-7        1.0
CONTAl  2     2650.   .17  1.00E-17  1.00E-17  1.00E-17   52.0   905.5
      1.83e-9  3.47e-5           1.          5.00e-04  5.00E-04
      7       0.4       0.3       1.          0.05
      7       0.4       0.3       1.E-5        1.0
BENTO   2     2650.   .40  1.00E-20  1.00E-20  1.00E-20   1.35   964.0
      3.58e-9  1.5e-5           1.          5.00e-04  5.00E-04
      7       0.4       0.3       1.          0.05
      7       0.4       0.3       5.6e-9        1.0
TOPBC   2     2650.   .12  1.00E-17  1.00E-17  1.00E-17   2.5   905.5
      1.83e-9  3.47e-5           1.          5.00e-04  5.00E-04
      7       0.4       0.5       1.          0.05
      7       0.4       0.5       5.6e-7        1.0
BOTBC   2     2650.   .12  1.00E-17  1.00E-17  1.00E-17   2.5   905.5
      1.83e-9  3.47e-5           1.          5.00e-04  5.00E-04
      7       0.4       0.5       1.          0.05
      7       0.4       0.5       5.6e-7        1.0

MULTI---1----2----3----4----5----6----7----8
      5       6       2       8
START---1----2----3----4----5----6----7----8
-----1 MOP: 123456789*123456789*1234 -----5-----6-----7-----8
PARAM---1----2----3----4----5----6----7----8
      39999  99991           4      5           9.8
      5.01728e+8  1.0e+3
      1.E-04   1.E+0           6.37E6  1.0e-3           0.0
                           0.0           25.0

```

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```
SELEC---1----2----3----4----5----6----7----8
      6       1       24      2
      -1.e5

      0.e-0   0.e-1
      0.e-9   0.e-9   1.e-5   0.0e-9   0.e-9   1.e-11
      1.8e11  14.0    1.e-5   1.0e-9               1.e-8
      1.0e30  14.0    1.e-5   1.0e-9               2.e-10

FOFT ---1----2----3----4----5----6----7----8
AE1 1
AO1 1

GENER---1----2----3----4----5----6----7----8
AL1 1AIR 1  4   1           COM5   3.0e-10
AM1 1AIR 1  4   1           COM5   3.0e-10
AN1 1AIR 1  4   1           COM5   3.0e-10
AO1 1AIR 1  4   1           COM5   3.0e-10
AP1 1AIR 1  4   1           COM5   3.0e-10
AQ1 1AIR 1  4   1           COM5   3.0e-10
AR1 1AIR 1  4   1           COM5   3.0e-10
AS1 1AIR 1  4   1           COM5   3.0e-10
AT1 1AIR 1  4   1           COM5   3.0e-10
AU1 1AIR 1  4   1           COM5   3.0e-10
AL1 1C14 1  4   1           COM3   1.0e-13
AM1 1C14 1  4   1           COM3   1.0e-13
AN1 1C14 1  4   1           COM3   1.0e-13
AO1 1C14 1  4   1           COM3   1.0e-13
AP1 1C14 1  4   1           COM3   1.0e-13
AQ1 1C14 1  4   1           COM3   1.0e-13
AR1 1C14 1  4   1           COM3   1.0e-13
AS1 1C14 1  4   1           COM3   1.0e-13
AT1 1C14 1  4   1           COM3   1.0e-13
AU1 1C14 1  4   1           COM3   1.0e-13
AL1 1HEAT 1 4   1           HEAT   1.00
...
```

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```

AM1 1HEA 1   4    1           HEAT      1.00
AN1 1HEA 1   4    1           HEAT      1.00
AO1 1HEA 1   4    1           HEAT      1.00
AP1 1HEA 1   4    1           HEAT      1.00
AQ1 1HEA 1   4    1           HEAT      1.00
AR1 1HEA 1   4    1           HEAT      1.00
AS1 1HEA 1   4    1           HEAT      1.00
AT1 1HEA 1   4    1           HEAT      1.00
AU1 1HEA 1   4    1           HEAT      1.00

INCON -- INITIAL CONDITIONS FOR 1251 ELEMENTS AT TIME  0.500000E+09
A21 1          0.12000536E+00
  0.6374000915391E+07 0.10000000000026E-02 0.5569126554103E-16 0.2331270365019E-18
  0.8664283833566E-20 0.2607711373189E+02
A31 1          0.12001080E+00
  0.6377999932395E+07 0.9999999999120E-03 0.1079403670680E-14 0.4211340455500E-17
  0.3980273919673E-18 0.2717146520376E+02
A41 1          0.12001639E+00
  0.6381998251120E+07 0.999999999951B-03 0.2046657817590E-13 0.7400076246940E-16
  0.1805346242483E-16 0.2830264322032E+02
A51 1          0.12002223E+00
  0.6385997247117E+07 0.1000000000444E-02 0.3788238250435E-12 0.1261076149346E-14
  0.8100797665784E-15 0.2949561382279E+02
A61 1          0.12002692E+00
  0.6388998954031E+07 0.9999999998392E-03 0.5207644024536E-11 0.1585693756698E-13
  0.3098439262167E-13 0.3046303591434E+02
A71 1          0.12003019E+00
  0.6391001188322E+07 0.9999999994434E-03 0.2850148282396E-10 0.8008835524733E-13
  0.4820218385785E-12 0.3114236594327E+02
A81 1          0.12003364E+00
  0.6393005107089E-07 0.1000000000125E-02 0.1568258500002E-09 0.4040533742984E-12
  0.7186702942244E-11 0.3186489833060B+02

```

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PART E (SimRad2_2.out)

TOUGH2 IS A PROGRAM FOR MULTIPHASE MULTICOMPONENT FLOW IN PERMEABLE MEDIA, INCLUDING HEAT FLOW. IT IS A MEMBER OF THE MULKOM FAMILY OF CODES, DEVELOPED AT LAWRENCE BERKELEY NATIONAL LABORATORY.

***** TOUGH2 - VERSION 2.0 (OCTOBER 1999) *****
***** T2CG2 Solver Package *****

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PARAMETERS FOR FLEXIBLE DIMENSIONING OF MAJOR ARRAYS (MAIN PROGRAM) ARE AS FOLLOWS

```
MNEL = 1500 MNCON = 5000 MNEQ = 6 MNK = 5 MNPH = 2 MNB = 8 MNODG = 300 MGTAB = 2000
```

```

MAXIMUM NUMBER OF VOLUME ELEMENTS (GRID BLOCKS): MNEL = 1500
MAXIMUM NUMBER OF CONNECTIONS (INTERFACES): MNCON = 5000
MAXIMUM LENGTH OF PRIMARY VARIABLE ARRAYS: MPROM = 9000
MAXIMUM NUMBER OF GENERATION ITEMS (SINKS/SOURCES): MNONG = 300
MAXIMUM NUMBER OF TABULAR (TIME-DEPENDENT) GENERATION DATA: MGTAB = 2000
LENGTH OF SECONDARY PARAMETER ARRAY: MSEI = 294000

```

LARGE LINEAR EQUATION ARRAYS: LENGTH OF IRN IS LIRN = 414000
LENGTH OF ICN AND CO IS LICN = 414000

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```

*****
*          EOS7R: EQUATION OF STATE FOR MIXTURES OF WATER/BRINE/RADIONUCLIDE(1)/RADIONUCLIDE(2)/AIR   *
*****
OPTIONS SELECTED ARE: (NN,NEQ,NPH,NB,NKIN) = (5,6,2,8,5)

NK    = 5 - NUMBER OF COMPONENTS
NEQ   = 6 - NUMBER OF EQUATIONS PER GRID BLOCK
NPH   = 2 - NUMBER OF PHASES THAT CAN BE PRESENT
NB    = 8 - NUMBER OF SECONDARY PARAMETERS OTHER THAN COMPONENT MASS FRACTIONS
NKIN  = 5 - NUMBER OF COMPONENTS FOR INITIALIZING THERMODYNAMIC CONDITIONS (default is NKIN = NK)

For NB = 6, diffusion is "off", for NB = 8, diffusion is "on"

AVAILABLE OPTIONS for (NN,NEQ,NPH,NB):
(5,5,2,6 or 8) - WATER, BRINE, RN1, RN2, AIR; ISOTHERMAL;           VARIABLES (P, XB, XRN1, XRN2, X OR S+10, T)
(5,6,2,6 or 8) - WATER, BRINE, RN1, RN2, AIR; NON-ISOTHERMAL;        VARIABLES (P, XB, XRN1, XRN2, X OR S+10, T)
(4,4,2,6 or 8) - WATER, BRINE, RN1, RN2, NO AIR; ISOTHERMAL;         VARIABLES (P, XB, XRN1, XRN2, T)
(4,5,2,6 or 8) - WATER, BRINE, RN1, RN2, NO AIR; NON-ISOTHERMAL;      VARIABLES (P, XB, XRN1, XRN2, T)

NKIN = NK or NKIN = NK-2. Default options are (5,5,2,8) - isothermal, diffusion "on", NKIN=NK

THE NK = 4 ("NO AIR") OPTIONS MAY ONLY BE USED FOR PROBLEMS WITH SINGLE-PHASE LIQUID CONDITIONS THROUGHOUT.

THE NORMAL NUMBER OF SECONDARY PARAMETERS OTHER THAN MASS FRACTIONS IS 6 PER PHASE. IN EOS7R, WE OPTIONAL ADD TO THIS A
SATURATION-DEPENDENT TORTUOSITY FOR EACH PHASE, AS WELL AS TEMPERATURE AND PRESSURE DEPENDENCE OF THE DIFFUSION COEFFICIENT.
*****
NKIN = 5 *** ALLOWS INITIALIZATION WITH DIFFERENT SETS OF PRIMARY VARIABLES. ***
*** THIS IS USEFUL FOR STARTING EOS7 SIMULATIONS FROM EOS7 INITIAL CONDITIONS. ***
= NK (default): (P,XB,XRN1,XRN2,XAIR,T) FOR SINGLE PHASE, (P,XB,XRN1,XRN2,S+10,T) FOR TWO-PHASE. (EOS7R FORMAT).
= NK-2: (P,XB,XAIR,T) FOR SINGLE PHASE, (P,XB,S+10,T) FOR TWO-PHASE. (EOS7 FORMAT). WILL INITIALIZE XRN1 = XRN2 = 0.
*****
THE PRIMARY VARIABLES ARE
P - PRESSURE   T - TEMPERATURE   XB - BRINE MASS FRACTION IN LIQUID (FOR SINGLE-PHASE GAS, XB IS BRINE MASS FRACTION IN GAS)
XRN1 - MASS FRACTION IN THE LIQUID OF RADIONUCLIDE(1) (PARENT)   XRN2 - MASS FRACTION IN THE LIQUID OF RADIONUCLIDE(2) (DAUGHTER)
S+10. - (GAS PHASE SATURATION + 10.)   X - AIR MASS FRACTION   T - TEMPERATURE

*****
*   COMPONENTS   *   *   FLUID PHASE CONDITION   PRIMARY VARIABLES   *
*****
*   # 1 - WATER   *   *   SINGLE-PHASE GAS (*)   P, XB, XRN1, XRN2, X, T   *
*   # 2 - BRINE   *   *   SINGLE-PHASE LIQUID (*)   P, XB, XRN1, XRN2, X, T   *
*   # 3 - RN1   *   *   TWO-PHASE (*)   P, XB, XRN1, XRN2, S+10., T   *
*   # 4 - RN2   *   *   *
*   # 5 - AIR   *   *   *
*   # 6 - HEAT   *   *   *

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*****
*   # 4 - RN2   *   *   *****
*   # 5 - AIR   *   *   (*) SINGLE-PHASE GAS NOT FULLY IMPLEMENTED.
*   # 6 - HEAT   *   *   (*) XRN1 AND XRN2 ARE ALWAYS MASS FRACTIONS IN THE AQUEOUS PHASE.
*   *
***** NEGATIVE REFERENCE PRESSURE OF -1.00000E+06 PA WAS SPECIFIED, THUS BRINE PROPERTIES ARE IDENTICAL TO WATER FOR ALL SALINITIES.
PROPERTIES OF THE RADIONUCLIDES: DOMAIN RADIONUCLIDE(1) RADIONUCLIDE(2)
HALF-LIFE (SECONDS): -ALL- 0.1800E+12 0.1000E+31
MOLECULAR WEIGHT (GM/MOLE): -ALL- 0.1400E+02 0.1400E+02
INVERSE HARM. CONST. (GM/PA): -ALL- 0.2000E-07 0.2000E-07
GAS SEPAR. DIFFUSIVITY (M**2/S): -ALL- 0.1000E+04 0.1000E+04
AQ. PHASE DIFFUSIVITY (M**2/S): -ALL- 0.1000E-08 0.1000E-08
DISTRIBUTION COEFF. (M**3/KG): CLAY 0.5000E-03 0.5000E-03
DISTRIBUTION COEFF. (M**3/KG): BENTO 0.5000E-03 0.5000E-03
DISTRIBUTION COEFF. (M**3/KG): TOPBC 0.5000E-03 0.5000E-03
DISTRIBUTION COEFF. (M**3/KG): BOTBC 0.5000E-03 0.5000E-03
MOLECULAR DIFFUSIVITY OF WATER, BRINE, XRN1, XRN2, AND AIR THROUGH THE GASEOUS AND AQUEOUS PHASES, (FDIAG(PHASE,COMP)) [M**2/S]:
PHASE 1 = GAS; PHASE 2 = AQUEOUS
PHASE COMP PHASE COMP
-1- -1- -2- -1- -3- -1- -4- -1- -5- -2- -1- -2- -2- -3- -2- -4- -2- -5-
0.00000E+00 0.00000E+00 0.10000E-04 0.10000E-04 0.00000E+00 0.00000E+00 0.10000E-08 0.10000E-08 0.10000E-10
***** VOLUME- AND MASS-BALANCES *****
***** [KCYC,ITER] = [ 46, 0 ] ***** THE TIME IS 0.500000E+09 SECONDS, OR 0.578704E+04 DAYS
***** PHASES PRESENT ***** COMPONENT MASS IN PLACE (KG)
***** PHASES   *   GAS   AQUEOUS   PHASES   *   GAS   AQUEOUS   ABSORBED   TOTAL   *****
***** PHASES   *   GAS   AQUEOUS   PHASES   *   GAS   AQUEOUS   ABSORBED   TOTAL   *****
***** VOLUME (M**3) * 0.45163332E-01 0.48327851E+01   COMPONENTS   *
MASS (KG) * 0.71172939E+01 0.48246059E+04   WATER * 0.27938157E-02 0.48193957E+04 0.00000000E+00 0.48193985E+04
***** ***** BRINE * 0.00000000E+00 0.48242227E+01 0.00000000E+00 0.48242227E+01
***** ***** RN1 * 0.53289383E-05 0.50246789E-03 0.19425825E-02 0.24973398E-02
***** ***** RN2 * 0.99866019E-06 0.37676413E-06 0.12409007E-05 0.26052222E-05
***** ***** AIR * 0.71144458E+01 0.38552179E+00 0.00000000E+00 0.74596768E+01
***** *****

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RADIONUCLIDE TRANSPORT PROBLEM

OUTPUT DATA AFTER (100, 7) -2-TIME STEPS

THE TIME IS 0.580704E+04 DAYS

TOTAL TIME	KCYC	ITERC	KON	DX1M	DX2M	DX3M	MAX. RES.	NER	KER	DELTEX	
0.501728E+09	100	7	604	2.0	0.40694E+06	0.76143E-06	0.37950E-08	0.57103E-05	397	1	0.53000E+05

ELEM.	INDEX	P (PA)	T (DEG-C)	SL	XBRINE(LIQ)	XRN1(LIQ)	XRN2(LIQ)	XAIRG	XRN1(GAS)	XRN2(GAS)	DL (KG/M**3)	
A21	1	0	0.64226E+07	0.26088E+02	0.10000E+01	0.10000E+02	0.61086E-16	0.25439E-18	0.75804E-10	0.18061E-11	0.37608E-12	0.99968E+03
A31	1	0	0.47558E+07	0.27159E+02	0.10000E+01	0.10000E+02	0.11898E-14	0.46145E-17	0.18481E-07	0.32959E-09	0.63912E-11	0.99940E+03
A41	1	0	0.63537E+07	0.28523E+02	0.10000E+01	0.10000E+02	0.22380E-14	0.16178E-17	0.18481E-07	0.38953E-09	0.63912E-11	0.99940E+03
A51	1	0	0.64226E+07	0.28523E+02	0.10000E+01	0.10000E+02	0.46828E-14	0.16178E-17	0.18481E-07	0.38953E-09	0.63912E-11	0.99940E+03
A61	1	5	0.66456E+07	0.30743E+02	0.10000E+01	0.10000E+02	0.56446E-11	0.17070E-13	0.68559E+00	0.11608E+00	0.17807E-07	0.99847E+03
A71	1	6	0.66940E+07	0.31240E+02	0.10000E+01	0.10000E+02	0.31225E-10	0.87213E-13	0.85656E+00	0.98148E-07	0.13707E-07	0.99826E+03
A81	1	7	0.67256E+07	0.31358E+02	0.10000E+01	0.10000E+02	0.17923E-09	0.53909E-12	0.99755E+00	0.89228E-08	0.13908E-08	0.99804E+03
A91	1	8	0.81317E+07	0.32790E+02	0.99986E+00	0.99986E+00	0.9326E-09	0.14154E-09	0.99962E+00	0.71408E-09	0.54184E-09	0.88398E+03
AA1	1	9	0.87129E+07	0.33736E+02	0.89975E+00	0.99860E+00	0.47125E-08	0.79132E-10	0.99638E+00	0.33638E-07	0.28242E-07	0.99834E+03
AB1	1	0	0.90502E+07	0.34428E+02	0.88308E+00	0.99858E+00	0.18154E-07	0.24119E-07	0.99962E+00	0.12489E-06	0.82958E-07	0.99823E+03
AC1	1	11	0.92851E+07	0.34549E+02	0.88308E+00	0.99858E+00	0.35913E-09	0.40183E-09	0.99962E+00	0.27358E-06	0.12085E-06	0.99813E+03
AD1	1	12	0.93605E+07	0.34660E+02	0.88308E+00	0.99858E+00	0.38705E-09	0.39770E-09	0.99962E+00	0.27358E-06	0.12085E-06	0.99813E+03
AE1	1	13	0.95766E+07	0.36213E+02	0.86172E+00	0.99848E+00	0.20274E-06	0.46187E-09	0.99961E+00	0.13016E-05	0.14826E-06	0.99788E+03
AF1	1	14	0.10022E+08	0.36377E+02	0.85616E+00	0.99839E+00	0.39016E-06	0.47848E-09	0.99961E+00	0.24240E-05	0.14862E-06	0.99774E+03
AG1	1	15	0.10567E+08	0.37943E+02	0.85186E+00	0.99830E+00	0.55739E-06	0.50368E-09	0.99961E+00	0.32843E-05	0.14839E-06	0.99761E+03
AH1	1	16	0.11036E+08	0.39061E+02	0.84785E+00	0.99823E+00	0.71885E-06	0.52509E-09	0.99960E+00	0.40558E-05	0.14813E-06	0.99739E+03
AI1	1	17	0.11438E+08	0.40278E+02	0.84309E+00	0.99816E+00	0.94149E-06	0.54307E-09	0.99959E+00	0.51267E-05	0.14787E-06	0.99709E+03
AJ1	1	18	0.11767E+08	0.41569E+02	0.83658E+00	0.99811E+00	0.12252E-05	0.55782E-09	0.99957E+00	0.64837E-05	0.14759E-06	0.99672E+03
AK1	1	19	0.12101E+08	0.42948E+02	0.83066E+00	0.99806E+00	0.18913E-05	0.57021E-09	0.99956E+00	0.78747E-05	0.14732E-05	0.99641E+03
AL1	1	20	0.12051E+08	0.43626E+02	0.44956E+00	0.99810E+00	0.17000E-05	0.59569E-09	0.99955E+00	0.87647E-05	0.14707E-05	0.99610E+03
AM1	1	21	0.12060E+08	0.43674E+02	0.45911E+00	0.99812E+00	0.17338E-05	0.57021E-09	0.99953E+00	0.89597E-05	0.14722E-06	0.99598E+03
AN1	1	22	0.12066E+08	0.43708E+02	0.52981E+00	0.99812E+00	0.17670E-05	0.57076E-09	0.99953E+00	0.91200E-05	0.14729E-06	0.99598E+03
AO1	1	23	0.12070E+08	0.43730E+02	0.54840E+00	0.99812E+00	0.17914E-05	0.57123E-09	0.99953E+00	0.92421E-05	0.14735E-06	0.99597E+03
AP1	1	24	0.12074E+08	0.43743E+02	0.55672E+00	0.99812E+00	0.18044E-05	0.57153E-09	0.99953E+00	0.93062E-05	0.14739E-06	0.99597E+03
AQ1	1	25	0.12077E+08	0.43745E+02	0.55668E+00	0.99812E+00	0.18040E-05	0.57162E-09	0.99953E+00	0.93023E-05	0.14737E-06	0.99597E+03
AR1	1	26	0.12079E+08	0.43747E+02	0.54879E+00	0.99812E+00	0.17904E-05	0.57151E-09	0.99953E+00	0.92302E-05	0.14732E-05	0.99597E+03
AS1	1	27	0.12081E+08	0.43750E+02	0.54879E+00	0.99812E+00	0.17904E-05	0.57121E-09	0.99953E+00	0.92302E-05	0.14724E-05	0.99598E+03
AT1	1	28	0.12083E+08	0.43752E+02	0.49454E+00	0.99812E+00	0.17231E-05	0.59556E-09	0.99953E+00	0.92335E-05	0.14716E-05	0.99599E+03
AU1	1	29	0.12082E+08	0.43659E+02	0.43237E+00	0.99812E+00	0.17014E-05	0.57099E-09	0.99953E+00	0.87697E-05	0.14715E-06	0.99601E+03
AV1	1	30	0.14332E+08	0.42876E+02	0.99854E+00	0.99971E+00	0.14460E-05	0.70703E-09	0.99962E+00	0.62835E-05	0.15362E-06	0.99729E+03
AW1	1	31	0.61676E+07	0.41385E+02	0.10000E+01	0.99917E+00	0.17027E-05	0.70225E-09	0.99903E+00	0.12855E-04	0.42107E-04	0.99459E+03
AX1	1	32	0.65636E+07	0.39954E+02	0.10000E+01	0.99974E+00	0.81278E-06	0.64553E-09	0.99718E+00	0.30679E-04	0.12183E-05	0.99513E+03
AY1	1	33	0.65223E+07	0.38594E+02	0.10000E+01	0.99939E-03	0.61958E-06	0.57052E-09	0.99030E+00	0.89291E-04	0.41111E-05	0.99563E+03

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